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JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH 2011-2012

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JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH 2011–2012

FOREWORD

The Centre has been actively contributing to the growth of scientific research in the country. Since inception in 1989, we have diversified from our initial focus on research in chemistry and physics of materials to biological and engineering sciences. While the primary focus of our Centre continues to be cutting-edge research both conceptually and technologically, we are also actively engaged in teaching and science outreach activities and also host a wide variety of scientific seminars, workshops and conferences of international standards. We continue to sponsor several programmes that enable Undergraduate and Master's students as well as teachers from all over the country to experience the joys of research by offering summer research fellowships and visiting fellowships, POCE and POBE.

With this brochure, we offer you a glimpse of the varied activities and achievements of the Centre and provide an overview of the diversity of opportunities for both students and scientists in the country and abroad.

Theoretical and empirical aspects of the design and synthesis of new and functionally unique materials ranging from solar cells to nanomaterials is the focus of research among several colleagues in the physical and chemical sciences, in addition to purely theoretical studies to gain basic understanding of the nature of physical interactions in the real world. Our faculty in the field of life sciences are engaged in tackling challenging questions as varied as the mysteries of behavioural and evolutionary aspects of living systems as also the genetic and molecular underpinnings of human diseases. The mechanics of the ebb and flow of fluids are explored by scientists interested in the dynamics of complex fluids and atmospheric forces. The geomorphological changes underlying landforms from the Himalayas to the Western Ghats form the topic of research of the Geodynamics Unit reflecting our scope that extends from the depths of the earth's crust to the lofty skies. In addition, we maintain the desire to embark on new and exciting research areas.

We believe in creating and sustaining an environment that fosters collaboration among these diverse fields of enquiry as evident from the many cross-discipline publications of our scientists. State-of-the art research facilities enable our scientists to work on areas of research that are on the threshold of new discoveries and compete with the best in the world. The scientific output of our faculty, in terms of publications, is among the highest in the country. Several of my colleagues have been awarded and recognised both internationally and nationally for their leadership in their respective research areas.

Our centre continues to receive support from the Department of Science and Technology (DST), Government of India and several other governmental and private sources. Some of our faculty are also recipients of foreign grants. Our small yet cosmopolitan nature enables the members of our community to effectively interact with each other, be it between students and faculty, administration or other support staff.

MRS Rao
President
JNCASR

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INTRODUCTION

"The real voyage of discovery consists not in seeking new landscapes, but in having new eyes."– Marcel Proust

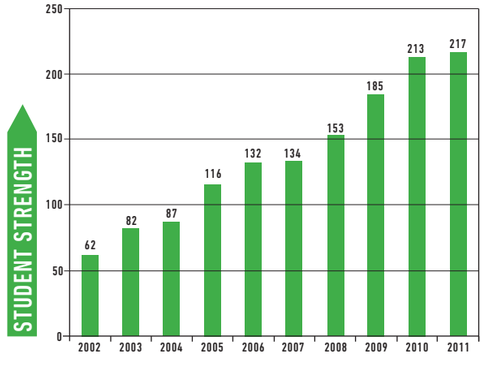
It is with these new eyes that the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) approaches science and engineering, with the undiluted intention of making discoveries that illuminate and improve all our lives.

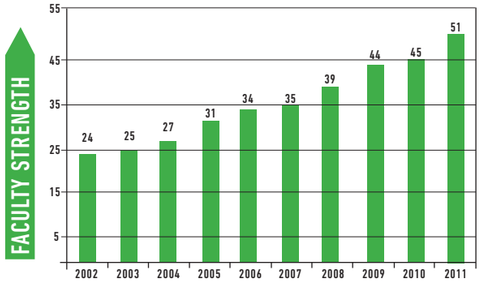
One of the country's leading multidisciplinary research institutions, JNCASR was instituted to commemorate the birth centenary of Pandit Jawaharlal Nehru in 1989. Its mandate was the relentless pursuit of cutting-edge scientific research. In its twenty-three years of existence, JNCASR has come to stand for insightful research of the highest level, and a deep commitment to science outreach.

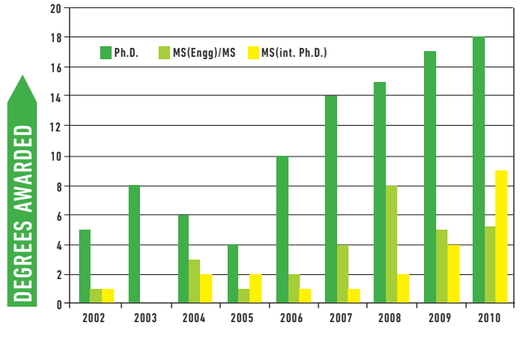
INSIGHTFUL RESEARCH

The spirit of scientific discovery has driven all the individual research units of the Centre to contribute significantly to their respective fields, by deepening the understanding of subjects as diverse as nanomaterials, fluid flows, material science, computational research, and molecular and evolutionary biology.

JNCASR researchers have published their findings in leading international scientific journals, and the number of these publications, too, has been steadily rising. A total of 86 students have received PhD degrees, and 31, MS degrees, over the last five years. While most of these young scientists have gone abroad for doctoral, or post-doctoral, research, many of these students have returned to India to take up positions in academia or industry.







The steadily-increasing number of patents filed by JNCASR is a further validation of the nature and impact of the work conducted at the Centre.

Of 66 patent applications filed, 12 have been granted, one design has been registered, and 5 inventions have been licensed. Members of the Centre's faculty have received international acclaim for their academic accomplishments. Prof CNR Rao holds the singular distinction of being elected Fellow of all the leading science academies in the world, while having received the Dan David Prize; the Queen's Medal of the Royal Society, London; the German Chemical Society's August-Wilhelm-von-Hoffmann-Denkmünze Medal; the Order of Friendship, Russia; the India Science Prize; and a host of other awards. The highly-recognised Prof Roddam Narasimha is a Fellow of the Royal Society of London; the National Science Academy, USA; and the recipient of prestigious awards like the Trieste Science Prize, Italy. Prof MRS Rao has received the Padma Sri Award from the Government of India. Other faculty members have also received acclaim and recognition, in the form of leading prizes like the Shanti Swaroop Bhatnagar Award; Fellowships of the Third World Academy of Sciences, the Indian Academy of Sciences, the National Academy of Sciences, the Indian National Science Academy, JC Bose, and Swarnajayanthi; the DAE Outstanding Research Career Award; the Materials Research Society of India Medal; the BM Birla Prize; the FICCI Award for Life Sciences; and the Young Asian Fluid Dynamicist Award.

INTERDISCIPLINARY COLLABORATION

The three key branches of research at the Centre are quite diverse: materials science (experimental and theoretical), fluid mechanics, and biology. The relative size of JNCASR, coupled with its active promotion of networking, and its very high faculty-to-student ratio (an astonishing 1:4), makes it a very fertile ground for cross-disciplinary collaboration. When a faculty belonging to the chemical, or physical, sciences collaborates with those immersed in the biological sciences, the result is a series of intra-JNCASR collaborations in novel interdisciplinary areas.

Collaborations such as these have even lead to the introduction of new research units. The New Chemistry Unit was established in 2008 to focus on the interdisciplinary aspects of chemical science, while the Nano Mission Council facilitated the creation of the Centre for Computational Materials Science in 2006. The Centre plans to initiate new cross-disciplinary research in the areas of Neurosciences, Soft Condensed Matter, and Physical Biology. Research on Advanced Materials is also being expanded.

JNCASR's International Centre for Materials Science, the first of its kind in India, has been facilitating collaboration and networking on a global scale, and has attracted some of the finest international talent since 2008. The Centre itself enjoys rich and active collaborations with institutions like the NIMS, Japan, and Purdue and Northwestern Universities, US. The Centre offers short-term visiting fellowships, and has received 21 international visitors as part of this programme. In turn, several scientists from ICMS have visited other leading institutes.

ICMS organises a highly successful annual International Materials Lecture by eminent scientists from all over the world. This series has already featured Prof. Tobin Marks, Northwestern University; Prof. Stuart Parkin, IBM Almaden Research Center; and Prof. Sir Richard Friend, Cavendish Laboratory, University of Cambridge. In the wake of its success, ICMS has also instituted an annual Materials Lecture that features leading eminent scientists, the first of which featured Prof Baldev Raj, President of the Indian National Academy of Engineering. In addition, nearly 35 seminars and special lectures have been held at the ICMS alone.

SCIENCE OUTREACH

JNCASR firmly believes in the criticality of science education for the development of scientific research. This translates into an abiding commitment to multiplying the outreach of science education, innovatively, and powerfully.

Existing programmes like the Summer Research Fellowships and Visiting Fellowships are being complemented by a slew of new programmes like Project-Oriented Biology Education (POBE). The Madan Mohan Malviya Amphitheatre and the CNR Rao Hall of Science on the campus are at the heart of the Centre's attempts at firing the scientific imagination of school students. The JNCASR series of monthly lectures have resulted in engagement with almost two thousand school students each year.

From sharing the joy of scientific discovery with school children, to providing a richly interconnected forum for the exchange of scientific thought, JNCASR is working towards building an inclusive, inspiring scientific community. From actively participating in the international community through published papers and patents, to focusing on advanced areas of research that will lead to solutions humanity has long sought after, the Centre is enabling discovery in key research fields. From the strict adherence to a small number of students, to the unbridled encouragement of student-faculty interaction and discussion, JNCASR is truly a place where one can worship at the altar of science.

FOUNDER CHAIR

CNR RAO
FRS, FASc, FNA, FTWAS, Hon FRSC, Hon F Inst P

CHAIR

S Balasubramanian
FASc

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Ranjan Datta*
Rajesh Ganapathy*
Sridhar Rajaram*

*Jointly with ICMS

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FNASc, FASc

SM Shivaprasad*
GU Kulkarni
Chandrabhas Narayana

HONORARY PROFESSOR

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FASc, FTWAS, FNASc (IISc, Bangalore)

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M Eswaramoorthy
Tapas Kumar Maji

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Swapan K Pati
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Srikanth Sastry
FNASc, FASc

Umesh V Waghmare
FNASc, FASc

NS Vidhyadhiraja

CHEMISTRY AND PHYSICS OF MATERIALS UNIT

Materials research in the Chemistry and Physics of Materials Unit (CPMU) spans a wide variety and includes work on nanomaterials, multifunctional materials, organic solar cells, hybrid materials, catalysts, optoelectronic materials and green solvents. The goal in these studies is the design and synthesis of novel architectures and its relationship to properties emanating thereof. Work on water splitting to generate hydrogen has also been initiated. The Unit's faculty are leaders in their chosen areas and have contributed substantially to both broadening the discipline and enriching it. The activities of the Unit are strengthened through close collaborations with associate members drawn from the International Centre for Materials Science and the Theoretical Sciences Unit.

Some of the recent highlights of our research are:
Efficient storage and release of hydrogen gas in graphene and materials derived from it, magnetism observed in nanoscopic forms of materials which are non-magnetic in bulk, magnetoelectric effect in a variety of oxides, a tri-colour sensing polymer device which is quite similar in its function to retinal cone cells, the synthesis and control of GaN nanostructures using molecular beam epitaxy, nanopatterning of a large number of compounds using single-source direct precursors through e-beam and soft lithography, the identification of key biochemical entities employing surface enhanced Raman spectroscopy, a novel pore-switching behaviour in porous layered carbon, synthesis of a chiral microporous solid from achiral linkers, and insights into the dissolution of cellulose in room temperature ionic liquids using advanced computer simulations.

The doctoral students of the Unit, currently numbering around forty five, are exposed to both the fundamentals of the subjects as well as to recent advances through a rigorous academic programme and technical seminars. Sixty five percent of them hold a fellowship granted by CSIR/UGC, based on their performance in the NET exam. The average time taken by a student of CPMU to submit her/his Ph.D. thesis is five years.

The Unit had taken a lead in offering an Integrated Ph.D. programme in Materials Science, in operation since 2007. Currently, thirty five such students are in various stages of this programme. The Unit is fully committed to teaching and to the development of human resource.

Six technical staff members of the Unit ably support the research activity not only in maintaining all the major experimental facilities, but also in finding innovative solutions to issues. The Unit also maintains a central workshop and a liquid nitrogen facility.

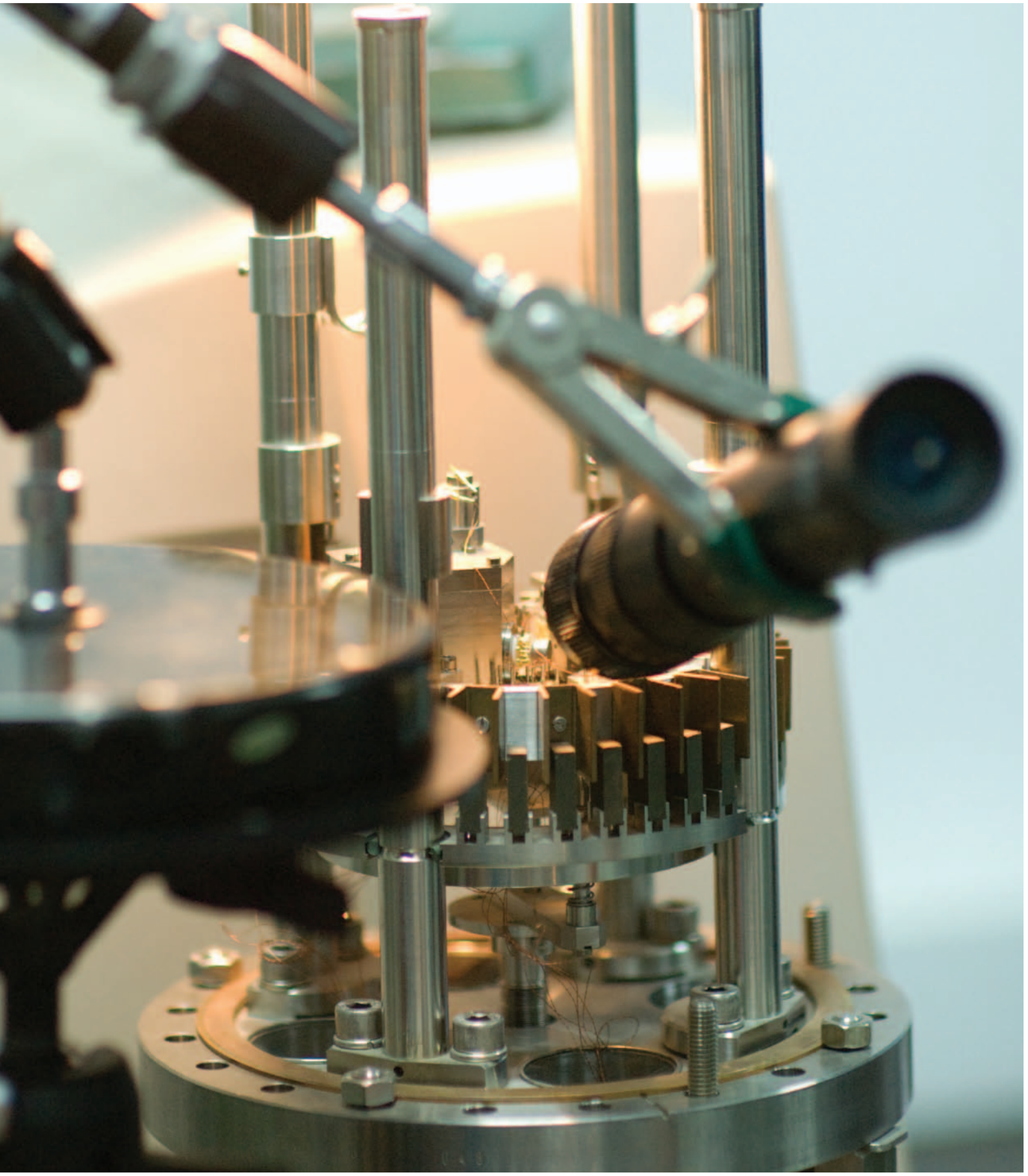
The following pages present the research interests and accomplishments of our core faculty. For further details, please visit: http://www.jncasr.ac.in/cpmu.

RECENT Ph.D. THESES

- Synthesis and direct patterning of functional nanostructures on flat and flexible substrates towards device fabrication (B Radha, 2012)
- Study of MBE growth and characterisation of Gallium Nitrate films and nanostructures (Manoj Kesaria, 2012)
- Investigations of structure-property relationships in functional metal-organic frameworks (Prakash Kanoo, 2011)
- Graphene (KS Subrahmanyam, 2011)
- Multiferroic properties and magnetization reversal in perovskite oxides (Pranab Mandal, 2011)
- Transport dynamics and fluctuations in active bulk heterojunction polymer solar cells (Monojit Bag, 2011)

RECENT Ph.D. THESES

- Nanoarchitecture: Morphogenesis and applications of nanostructured materials (Katla Sai Krishna, 2011)
- Study of the role of superstructural phases and interfacial properties on the growth of InN films (K Jithesh, 2011)
- Inelastic light scattering investigations on novel materials (Gopal K Pradhan, 2010)
- Molecular dynamics simulation studies on the structure, dynamics, and interfacial properties of room temperature ionic liquids (Soumya Saswati Sarangi, 2010)



CPMU FACILITIES

- Single Crystal X-ray diffractometer with CCD facility (Bruker)
- ESCA facility with UVPS, and LEED
- Pulsed laser reactive ablation apparatus attached with mass spectrometer
- Scanning Tunneling and Atomic Force Microscopes (STM/AFM) operating in air and at low temperature
- Variable Temperature STM
- Catalyst characterization with Gas chromatograph
- Quadrupole Mass Spectrometer and Residual Gas Analyzer
- Carbon arc-discharge Unit
- Large number of furnaces for making samples in various atmospheres in the range 300°C to 1700°C
- A closed cycle cryocooled 15 T superconducting magnet with a room temperature bore and an optical window
- Floating zone melting crystal growth apparatus
- High Resolution Transmission Electron Microscope (HRTEM) (300 kV, JEOL 3010)
- Scanning Electron Microscope (SEM) with EDAX (Leica¬440I)
- Magnetometer (VSM) and Faraday balance
- Surface area measuring apparatus
- Powder X-ray diffractometers (Bruker, Siefert and Mini Rigaku)
- Four Probe conductivity setup (15 K-325 K)
- Fourier Transform Infra-red Spectrometer to operate in the 200-7500 cm-1 range along with DRIFTS, environmental cells (77 K to 523 K)) (Bruker) for controlled studies
- Thermal characterization up to 1250 K (Mettler)
- UV-VIS spectrometer (Perkin-Elmer)
- Fluorescence spectrometer (Perkin-Elmer)
- Mössbauer Spectrometer
- Brillouin Spectrometer
- Micro and Indigenously built Raman Spectrometers
- Crystal polishing instrument
- Diamond anvil cell for high pressure research
- Optical stereo microscope with 200X magnification
- Low temperature compressed Helium cryostat
- Glove Box (< 2 ppm O_2 and H_2O environment) integrated with spin coating unit and accessories for device fabrication
- Fabrication facilities for Light emitting diode (LED), photovoltaic (PV) diodes and solar cells, field effect transistor (FET)
- Beowulf clusters for computational research
- Device LED, PV, FET measurement facilities
- Soft-lithography and Photolithography Implementation facilities
- Time (> 10 ns) and spatially (~ 50 nm) resolved photocurrent measurements
- Photolumiscence emission and excitation spectroscopy
- Physical Property Measuring System (PPMS, Quantum Design, USA) Evercool with 9T magnet (options: AC/DC susceptibility, AC/DC transport and heat capacity)
- RF magnetron sputtering for making thin films and superlattices
- Chemisorption - Physisorption Analyzer - Quantachrome Autosorb®-1-C
- Zetasizer Nano ZS particle size analyzer - Malvern instruments
- Precision Workstation (Radiant Technologies Inc) for dielectric measurements
- Near-field Scanning optical microscope
- Field Emission Scanning Electron Microscope with EDAX and E-beam lithography.
- Nano Probe Station
- Thin Film XRD
- Small angle X-ray scattering (NANOSTAR - Bruker)

S Balasubramanian

BALASUBRAMANIAN SUNDARAM RECEIVED HIS Ph.D. IN CHEMICAL SCIENCES FROM THE INDIAN INSTITUTE OF SCIENCE. HE WAS A POST-DOCTORAL FELLOW IN CHEMISTRY AT THE UNIVERSITY OF PENNSYLVANIA BEFORE JOINING JNCASR IN 1998.

MOLECULAR MODELLING OF MATERIALS

Our research is focused on molecular interactions and their role in the organization of molecules in condensed systems. We study crystalline and amorphous solids, liquids, supercritical fluids, interfaces, biological, and complex chemical systems using Molecular Dynamics (MD) methods. Realistic modelling of materials can enable one to obtain insight into microscopic processes that underlie experimental observations, and computational techniques such as MD provide us with such details. We employ two flavours of the MD technique: Classical Molecular Dynamics based on empirical interaction potentials, and *ab initio* Molecular Dynamics (AIMD) using quantum density functional theory.

Recent activities include the prediction of the crystal structure of carbonic acid, a compound of increasing environmental interest. This work involved the use of an array of advanced simulation techniques and a precise comparison to experimentally-known vibrational spectrum. Modelling supramolecular polymerization and self-assembly of chemically relevant molecules is another area that we have embarked on. Storage of gases such as carbon dioxide and hydrogen in solids and liquids is an active area of research in our Group. Our work focuses not only on the microscopic interactions responsible for gas adsorption but also on the prediction of adsorption isotherms using advanced Monte Carlo methods.

We routinely develop large codes to carry out these simulations on supercomputers. We work closely with experimental groups on campus and elsewhere.

KEY PUBLICATIONS

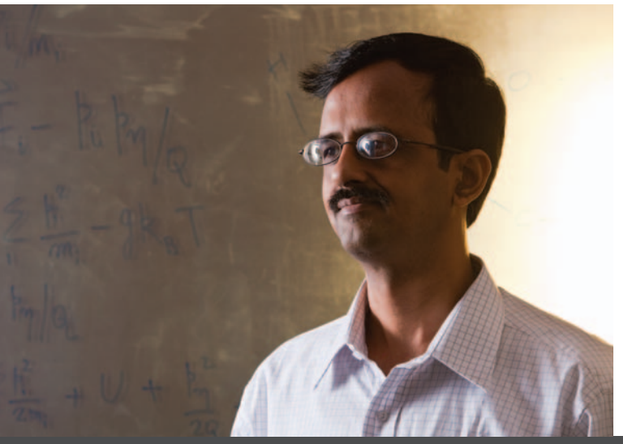
RS Payal, R Bharath, G Periyasamy, and S Balasubramanian, *Density functional theory investigations on the structure and dissolution mechanisms for cellobiose and xylan in an ionic liquid: Gas phase and cluster calculations,* **Journal of Physical Chemistry B 116,** 833-840 (2012).

SK Reddy, CH Kulkarni, and S Balasubramanian, *Theoretical investigations of candidate crystal structures for ß-carbonic acid,* **Journal of Chemical Physics 134,** 124511 (2011).

SS Sarangi, SK Reddy, and S Balasubramanian, *Low-Frequency vibrational modes of room temperature ionic liquids,* **Journal of Physical Chemistry B 115,** 1874-1880 (2011).

SG Raju, and S Balasubramanian, *Emergence of nanoscale order in room temperature ionic liquids: Simulation of symmetric 1, 3-didecylimidazolium hexafluorophosphate,* **Journal of Materials Chemistry 19,** 4343-4347 (2009).

BL Bhargava, and S Balasubramanian, *A refined potential model for atomistic simulations of an ionic liquid, [bmim][PF6],* **Journal of Chemical Physics 127,** 114510 (2007).



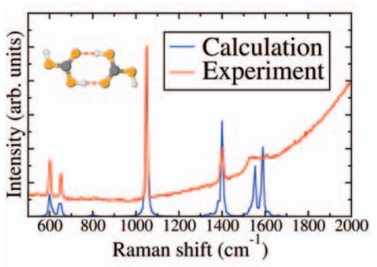


Fig. : Prediction of molecular motifs in crystalline ß-carbonic acid. Computer simulations reveal that the solid is constituted by linearly hydrogen bonded monomers

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M ESWARAMOORTHY OBTAINED HIS PHD FROM ANNA UNIVERSITY. HE WAS A POST-DOCTORAL FELLOW AT AIST, JAPAN, AND BRISTOL UNIVERSITY, UK, BEFORE JOINING JNCASR AS A FACULTY FELLOW.

NANOMATERIALS AND CATALYSIS

Our Group's research work focuses on the following areas: morphogenesis, intracellular drug delivery, nanocomposites, porous materials, and catalysis. Some of the specific problems being pursued in our Group related to these areas are briefly described here.

MORPHOGENESIS: SHAPING OF NANOMATERIALS

Nature, the doyen of science, constructs complex functional materials with hierarchial architectures. Horns or bones, shells or skulls, it selectively picks up the bricks – the requisite building blocks – from organic or inorganic components, and organises them in a programmed manner. Over a period of evolution, it learnt the art of intertwining organics and inorganics in an impeccable way to make light, yet tough materials and pass on this trick from generation to generation. Many times, it elegantly uses the vesicles made up of lipid bilayers as the reaction containers to make biominerals with defined shapes which defy the rules of thermodynamics. Taking a leaf out of Nature's book, we are attempting to make materials in different forms such as tubes, rings, spheres, and cups, by self-assembly and template-based methods.

MATERIALS FOR INTRACELLULAR DRUG DELIVERY

We have also embarked on the identification and development of new, functional nanomaterials for intracellular drug delivery. Developing such intracellular carriers that have no barriers across the cell membranes and nuclear membranes could find potential therapeutic applications. We have found that glucose-derived carbon nanospheres are intrinsically fluorescent, and can be used as a carrier for nuclear delivery.

CATALYSIS

Catalysis using porous materials is important, both, from the shape-selective, as well as the green chemistry points of view. Porous nanomaterials and metal/ metal oxide nanoparticles synthesized in our laboratory will be used to test some catalytic reactions like NOx removal, methane conversion, and selective oxidation of hydrocarbons.

KEY PUBLICATIONS

KKR Datta, D Jagadeesan, C Kulkarni, A Kamath, R Datta, and M Eswaramoorthy, *Observation of Pore-switching Behaviour in Porous Layered Carbon through Mesoscale Order-Disorder Transformation,* **Angew. Chem. Int. Ed. 50,** 3929-3933 (2011).

KV Rao, KKR. Datta, M Eswaramoorthy, and SJ George, *Light-Harvesting Hybrid Hydrogels: Energy Transfer Induced Amplified Fluorescence in Non-Covalently Assembled Chromophore-Organoclay Composites,* **Angew. Chem. Int. Ed. 50,** 1179-1184 (2011).

K Sai Krishna, CSS Sandeep, Reji Philip, and M Eswaramoorthy, *Mixing does the magic: A rapid synthesis of high surface area noble metal nanosponges showing broadband nonlinear optical response,* **ACS Nano 4,** 2681-2688 (2010).

C Piyush, J Dinesh, and M Eswaramoorthy, *pH sensitive breathing of clay within the polyelectrolyte matrix,* **ACS Nano 4,** 5921-5929 (2010).

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GU KULKARNI OBTAINED HIS Ph.D. IN SOLID STATE CHEMISTRY FROM THE INDIAN INSTITUTE OF SCIENCE. HE WAS A POST-DOCTORAL FELLOW IN CHEMISTRY AT CARDIFF UNIVERSITY BEFORE JOINING JNCASR IN 1995.

NANOMATERIALS, NANOFABRICATION, MOLECULAR CRYSTALS

Our main theme of research is studying matter at the Nanoscale. When the size of a material is reduced to a length scale typical of the interactions therein, quantum confinement of electrons sets in, leading to unusual properties that depend on the size of the system itself. This explains the growing interest in both academic and industrial circles to synthesize new nanomaterials with tailor made properties.

Our research interests are focused on nanocrystalline metal and semiconductor films, exotic nanostructures from pulsed laser deposition, the patterned synthesis of nanomaterials and nanodevice fabrication, and the structure and photophysical properties of molecular crystals.

INNOVATIVE METHODS FOR DIRECT WRITE NANOLITHOGRAPHY

An important and widely pursued aspect of nanopatterning is related to casting metals into submicrometer features and their exploitation as interconnects, solder in nanocircuitry, sensor elements, or catalysts to grow nanotubes and nanorods. In this activity, direct write precursors have been developed, which enable us to produce metal and semiconductor features in a single step by e-beam lithography and soft lithography. Electrostatic nanolithography using biased atomic force microscope (AFM) tip has been applied to pattern functional materials on polymeric films.

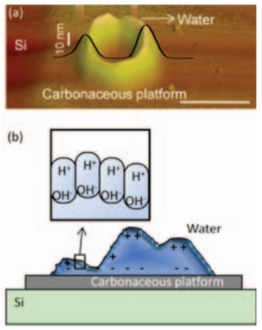

Fig. : Electrocondensation and evaporation of attoliter water droplets: Direct visualization using AFM
(a)The topography image and corresponding height profile of a water pattern showing unusually sharp morphology (Scale bar, 2 μm).
(b) AFM tip-induced charge and polarization contribute to the anomalous droplet shapes and the evaporation characteristics observed (N Kurra, A Scott, GU Kulkarni, Nano Research, 2010)

SELF-ASSEMBLED AND SOLDERED CARBON NANOTUBES IN CIRCUITS

Carbon nanotubes are considered too large for chemical manipulation and rather small for mechanical grippers. For instance, it is not easy to manipulate and arrange CNTs in a circuit. We have used a metal organic precursor to direct the self-assembly of individual CNTs across gap electrodes. This is done by patterning the precursor along the gap electrodes by e-beam lithography. The CNTs assemble in a highly desirable configuration.

Thermal activation of the precursor leads to metallization and thus, the insitu soldering of the CNTs. The resulting contacts are ohmic in nature. The resistive fuse action of insitu soldered CNTs is observed as well. Other highlights include surface-enhanced Raman scattering (SERS) substrates and Raman chip fabrication, highly robust metal-polymer composites, phenyleneethynylene-based molecular crystals-relating structure and photophysical properties.

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TAPAS KUMAR MAJI OBTAINED HIS Ph.D. IN INORGANIC CHEMISTRY FROM THE INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE (IACS), JADAVPUR UNIVERSITY, IN 2002. HE DID POST-DOCTORAL RESEARCH AT KYOTO UNIVERSITY, JAPAN, AND WAS LECTURER IN CHEMISTRY, JADAVPUR UNIVERSITY, BEFORE JOINING JNCASR IN 2006.

FUNCTIONAL MATERIALS BASED ON METAL-ORGANIC FRAMEWORKS (MOFs)

Our research work is focused on the new strategies for the synthesis of solid state materials that addresses the contemporary problem related to energy and environment. We are engaged in the synthetic aspects and design of metal-organic (hybrid) frameworks (MOFs) or porous coordination polymers (PCPs) for wide range applications like gas storage (H_2, CO_2, CH_4, etc), separation, magnetism, catalysis, sensing and light harvesting (Fig.1).

We also looked at magnetic property of this hybrid system mainly focusing on molecular porous magnets and guest induced modulation of Tc. Introducing functional groups in the pores in MOFs has been one of the key aspects of our research and we have been successful to make materials that show interesting catalytic (heterogeneous) and selective gas uptake characteristics. We also study excited state photophysical properties of these hybrid materials with the ultimate goal of white light emission and artificial photosynthetic system (Light harvesting). We are also concern about the processibility issues of these hybrid materials and started fabricating MOFs at nanoscale.

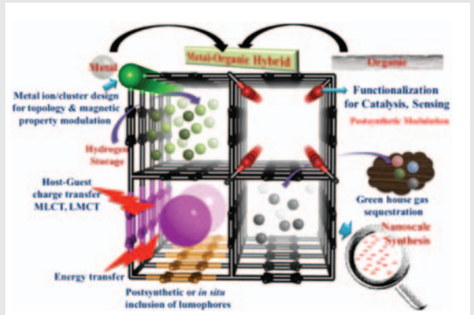

Fig. 1: Multifunctional MOFs

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Nivedita Sikdar

K S Narayan

KS NARAYAN OBTAINED HIS PHD IN CONDENSED MATTER PHYSICS FROM THE OHIO STATE UNIVERSITY IN 1991. HE WAS A SCIENTIST AT WRIGHT PATTERSON AIR FORCE BASE BEFORE JOINING JNCASR IN 1994. HE IS A FELLOW OF THE INDIAN ACADEMY OF SCIENCE, AND NATIONAL ACADEMY OF SCIENCE, INDIA.

ORGANIC ELECTRONICS: DEVICE PHYSICS & PHOTOPHYSICS

ORGANIC SOLAR CELLS: Device fabrication, measurement, and analysis.
POLYMERIC FIELD EFFECT TRANSISTORS: High k effects, and switching.
BIOELECTRONICS: Optoelectronic studies of retinal tissue and integration with conducting polymers, stem cell differentiation on electroactive substrates.
MICROSCOPY: Near field scanning microscopy (NSOM) and force microscopy of photoactive semiconducting polymers, and optical phenomena in confined structures fabricated using soft matter lithography procedures.

SOME NOTEWORTHY CONTRIBUTIONS FROM THE LABORATORY IN THE PAST ARE LISTED BELOW:

- Polymer photo field effect transistors
- Efficient plastic solar cells
- Synergistic processes at bacteriorhodopsin-conducting polymer interface
- Flexible polymer-based light position sensor spanning sub-micron to few mm range
- High-resolution photocurrent imaging for estimating transport length scales and identifying active regions
- Noise measurements to understand defects and degradation in organic solar cells

KEY PUBLICATIONS

Monojit Bag, NS Vidhyadhiraja and KS Narayan, *Fluctuations in Photocurrent of Bulk Heterojunction Polymor Solar Cells - A Valuable tool to understand microscopic and degradation processes,* **Applied Physics Letters, 101,** 043903 (2012).

S Mukhopadhyay and KS Narayan, *Rationalization of donor-acceptor ratio in bulk heterojunction solar cells using lateral photocurrent studies,* **Applied Physics Letters, 100,** 166305-166305 (2012).

Satyaprasad Senanayak, Suchismita Guha and KS Narayan, *Polarization fluctuation dominated electrical transport processes of polymor-based ferroelectric field effect transistors,* **Physical Review B, 85,** 115311 (2012).

Vini Gautam, Monojit Bag, and KS Narayan, Single-Pixel, *Single-Layer Polymer Device as a Tri-color Sensor with Signals Mimicking Natural Photoreceptors,* **Journal of the American Chemical Society 133,** 17942-17949 (2011).

V Vijay, D Arun, and KS Narayan, *In-situ Studies of Strain Dependent Transport Properties of Conducting Polymers on Elastomeric Substrates,* **Journal of Applied Physics 109,** 84525-6 (2011).

Sabyasachi Mukhopadhyay, Srinidhi Ramachandra and K. S. Narayan, *Direct Observation of Charge Generating Regions and Transport Pathways in Bulk Heterojunction Solar Cells with Asymmetric Electrodes using Near Field Photocurrent Microscopy,* **Journal of Physical Chemistry C, 115,** 17184 (2011).

Anshuman J Das, Clement Lafargue, Melanie Lebental, Joseph Zyss and KS Narayan, *Three-dimensional microlasers based on polymer fibers fabricated by electrospinning,* **Applied Physics Letters, 99,** 263303 (2011).

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INTEGRATED Ph.D. STUDENT
Prashanth

Chandrabhas Narayana

CHANDRABHAS NARAYANA RECEIVED HIS Ph.D. IN PHYSICS FROM THE INDIAN INSTITUTE OF SCIENCE, BANGALORE, AND WENT ON TO DO POST-DOCTORAL RESEARCH AT CORNELL UNIVERSITY, ITHACA, NEW YORK, USA IN THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING. HE HAS BEEN A PART OF THE CHEMISTRY AND PHYSICS OF MATERIALS UNIT, JNCASR, FROM 1998.

RAMAN AND BRILLOUIN SPECTROSCOPY, HIGH PRESSURE RESEARCH IN THE STUDY OF MATERIALS

Raman spectroscopy is an integral part of research carried out in our Light Scattering Laboratory (LSL). Initially, Raman spectroscopy was mostly used to study materials with an interest in understanding the physics of these materials. However, it was soon necessary to look at materials in the chemical and biological world, too. Surface-enhanced Raman spectroscopy (SERS) has been employed by us to understand biological systems.

Due to the nature of our collaborations, our Group looks at two important aspects. It has been seen that in the absence of x-ray crystallographic data on proteins, drug discovery has suffered. Our Group, in collaboration with Prof. Tapas K Kundu's group, has demonstrated that SERS can be effectively used to study small molecule-protein interactions.

In the quest for better SERS materials, and to use it as a potential tool for DNA/ RNA detection without PCR amplification, the Group has developed many SERS active materials. We, alongwith Prof. Ranga Udaykumar, have demonstrated that up to a few hundreds of RNA copies can be detected without PCR amplification in the case of HIV strains. The technique has entered the national phase of the patent. We are the first group to demonstrate the use of SERS as a drug designing tool along with Prof. Tapas K Kundu's group.

Our Group also uses Brillouin Spectroscopy to study the elastic, magnetic and molecular properties of materials, and is the only one of its kind in India. Currently the Group is developing a micro-Brillouin setup to study acoustic phonons in nanosystems under the application of electric fields. It is an important area of research which aids the device fabricators with the knowledge of the mechanical strength of nanomaterials in actual applications.

The LSL Group also uses high pressure to study material properties to understand the underlying phenomenon, like multi-ferroics, and ionic conductors. Raman and synchrotron x-ray studies are performed to elucidate these properties under pressure. We have set up the high pressure beamlines at, both, INDUS, RRCAT, Indore, and Photon Factory, KEK, Tsukuba, Japan. The Group has published over 75 publications, and has national and international (three each) patents.

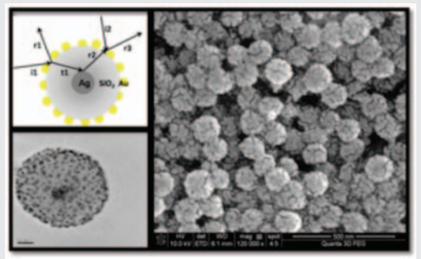

Fig. : FESEM, TEM and schematics of gold, silica, silver core-shell nanostructure for SERS applications

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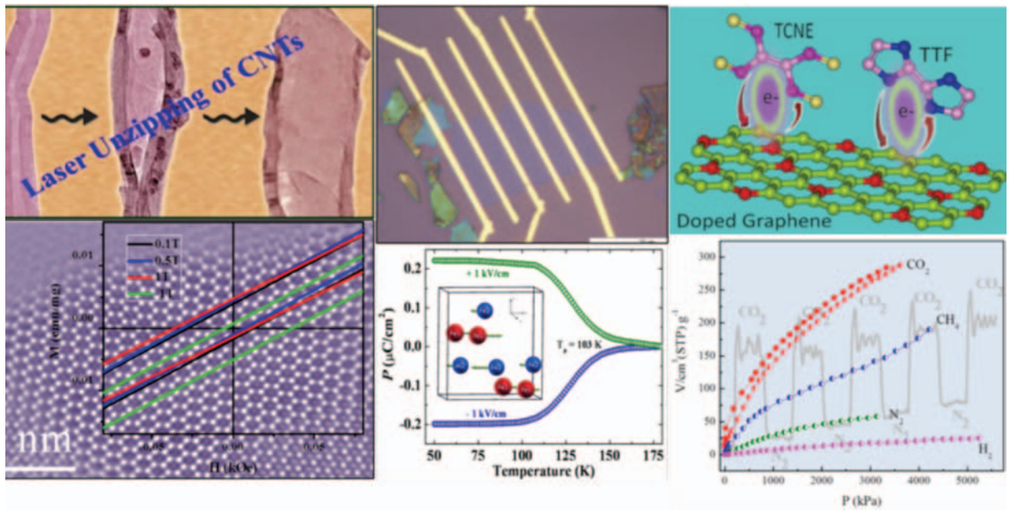
C N R Rao

CNR RAO, D.Sc. (MYSORE), Ph.D. (PURDUE), Sc.D. (HC), D.Sc. (HC), L.L.D. (HC), D.LITT. (HC), F.R.S., HON. F.R.S.C., HON. F. INST. P. IS A NATIONAL RESEARCH PROFESSOR AND FOUNDER AND HONORARY PRESIDENT OF JNCASR. HE IS ALSO THE DIRECTOR OF THE INTERNATIONAL CENTRE FOR MATERIALS SCIENCE (ICMS).

CHEMISTRY OF MATERIALS

The group's research centers on understanding various fundamental and technologically important aspects of nanoscience. The main focus is on the development of new approaches for the large scale synthesis of various carbon nanostructures like nanotubes, graphene and graphene-nanoribbons and scrolls with special emphasis on their properties and applications. New strategies are being pursued to prepare exotic graphene analogues of inorganic layered materials and borocarbonitrides. A part of the activity includes gaining insight into multiferroic and magnetoelectric oxides. One of the most recent interests of the group is to develop new catalysts for hydrogen generation by water splitting.



S M Shivaprasad

HE OBTAINED MASTERS AND Ph.D. IN PHYSICS FROM KARNATAKA UNIVERSITY, FOLLOWED BY POST DOCTORAL RESEARCH AT IIT DELHI AND UNIVERSITY OF SUSSEX. HE WAS A VISITING SCIENTIST AT NIST, USA, RUTGERS UNIVERSITY, TOHOKU UNIVERSITY AND UNIVERSITY OF ULM. HE SERVED NPL, NEW-DELHI BEFORE JOINING JNCASR IN 2007. HE HAS BEEN THE RECIPIENT OF THE CSIR YOUNG SCIENTIST AWARD, OUTSTANDING RESEARCHER AWARD, MRSI-ICSC ANNUAL PRIZE, MRSI MEDAL, RAK-CAM SENIOR FELLOWSHIP AND CNR RAO ORATION AWARD.

EPITAXY AND NANOSTRUCTURES

1. EPITAXIAL GROWTH OF III-NITRIDE FILMS AND NANOSTRUCTURES:
Our's is an experimental group that studies the formation of interfaces and thin films, of epitaxial and nanostructured films. We are motivated by the need to modify Gp-III nitride thin films for high performance optoelectronic devices by exploiting epitaxy and low-dimensional properties. We employ techniques like Molecular Beam Epitaxy, RHEED/LEED, Ellipsometry, XPS, CL/PL, HRXRD, FESEM/HR-TEM, etc for growth and characterization.

We have developed a novel approach of Superlattice Matching Epitaxy to form stable superstructural submonolayer phases by adsorption of metal adatom on Si(111) & Si(100) surfaces and use them as templates to grow high quality GaN and InN 2D films with low defect density and excellent optoelectronic properties. Kinetically controlled retarded epitaxial growth is used to form high density of self ordered and non-catalytic spontaneous growth of nanostructures. The GaN adsorption is kinetically driven to form faceted wurtzite self-organized nanorods and nanotubes with very interesting optoelectronic properties. The ordered GaN c-oriented GaN nanowall network, formed under nitrogen rich conditions has length scales that depends on growth conditions. We have observed a very strong photoluminescence enhancement due to Plasmon-coupling with metal nanoparticles, coherent emission due to confinement in the spontaneously formed cavities and confinement induced magnetism. We also address the issue of Moss-Burstein Shift to explain the band gap variation observed in InN films.

2. METAL/SEMICONDUCTOR INTERFACE:
We also perform surface science experiments of sub-monolayer adsorption of Gp III metal on Silicon surfaces of various orientations and reconstructions. We have explored several aspects of the Si(100) and Si(111) surfaces and high index Si(5 5 12) which has interesting 1-D faceted grooves enabling formation of single atom wide nanowire. We form 2D-superstructural phase diagram of different structural and electronic properties. These submonolayer phases are used as templates for growing epitaxial films and nanostructures.

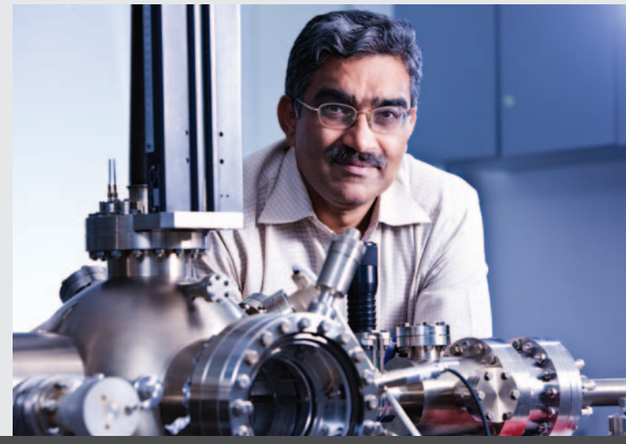
KEY PUBLICATIONS

Role of native defects in nitrogen flux dependent carrier concentration of InN films grown by MBE, **Journal of Applied Physics, 112(7),** 073510 (2012)

Dependence of crystal orientation and bandgap on substrate temperature of molecular-beam epitaxy grown InN on bare Al_2O_3 (0001)" **Journal of Applied Physics, 109** (2011) 093513

Evidence for Dislocation Induced Spontaneous Formation of GaN Nanowalls and Nanocolumns on Bare C-Plane Sapphire", **ACS Journal of Crystal Growth and Design, 11** (2011) 4900

Nitrogen flux induced GaN nanostructure nucleation at misfit dislocations on Al2O3(0001), **Applied Physics Letters, 99** (2011) 143105



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A Sundaresan

A SUNDARESAN HAS OBTAINED HIS Ph.D. IN CHEMISTRY FROM IIT BOMBAY IN 1994. HE WAS A POST-DOCTORAL FELLOW AT LABORATOIRE CRYSTALLOGRAPHY, CAEN; INVITED RESEARCHER, LEPES, CNRS, GRENOBLE, FRANCE; AND RESEARCHER, JST-CREST, AIST TSUKUBA, JAPAN, BEFORE JOINING JNCASR IN 2004.

MAGNETISM, SUPERCONDUCTIVITY AND MULTIFERROICITY

The main focus of his research is to understand the relationship between structure and properties of materials. This involves both fundamental and applied aspects of chemistry and physics of solid state, and a spectrum of materials including superconductors, multiferroics and magnetic materials. While continuing to work on bulk and thin film materials, he and his collaborators have recently discovered magnetism in otherwise nonmagnetic inorganic materials at the nanoscale, and suggested that ferromagnetism is a rather universal phenomenon of nano-sized inorganic materials.

SURFACE FERROMAGNETISM

The nonmagnetic oxides such as CeO_2, Al_2O_3, ZnO, In_2O_3, SnO_2 and MgO become a weak ferromagnet at room temperature when they are made at the nanoscale. The origin of this unexpected ferromagnetism has been shown to be confined only to the surface of the nanoparticles and suggested to be in the anion and/or cation vacancies at the surface. Based on this work, the ferromagnetism of nanoparticles was suggested to be universal feature not only of oxides but also of nitrides and chalcogenides. With its origin in the surface of nanoparticles, it was proposed that such ferromagnetism could coexist with any other functional properties of the bulk form. While incompatible with superconductivity, such ferromagnetism was demonstrated in the normal state of metal oxide and nitride superconductors.

MAGNETIZATION REVERSAL IN $AFE_{0.5}MN_{0.5}O_3$ (A=BI,Y & GD) PEROVSKITE

Investigations on B-site disordered perovskite $AFe_{0.5}Mn_{0.5}O_3$ showed interesting magnetic properties. For example, the compound $BiFe_{0.5}Mn_{0.5}O_3$ exhibits magnetic ordering at high temperature (TN= 270 K). Below TN, the magnetization under low applied field (50 Oe) changes sign below certain temperature (T*) and remains negative down to low temperature. On the other hand, under negative applied field (-50 Oe) the magnetization becomes positive below T*. Similar B-site disordered perovskite, for example, $AFe_{1-x}CrO_3$, has been studied and the origin of magnetization reversal is understood based on ferrimagnetic grounds state arising from antiferromagnetic coupling of Fe-Fe, Cr-Cr and Fe-Cr canted moments.

MULTIFERROICS

Multiferroics are materials that exhibit magnetism and ferroelectricity simultaneously. Magnetoelectric multiferroics are an interesting class of materials because the coupling of the two order parameters leads to new device application through the control of magnetism by an applied electric field, and control of electric polarization by an applied magnetic field. Two new families of magnetoelectric multiferroic materials, namely, $YFe_{1-x}M_xO_3$ (M=Mn and Cr) and $RCrO_3$ (R=magnetic rare-earth) are discovered. Though the crystal structure of these materials is centrosymmetric (Pnma), the ferroelectricity in the former appears due to spin-disorder whereas in the later it originates from magnetic interactions between rare-earth and chromium ions.

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MS STUDENT
Chandan De

MEMBERS

Prof V Krishnan
Mrs Indumati Rao
Ms Jatinder Kaur
Mr Sanjay SR Rao

EDUCATION TECHNOLOGY UNIT

ETU

Education Technology Unit was established in 1996. The focus of the unit is to develop learning and teaching materials. It has developed and produced multimedia CD-ROMs in various science subjects in different languages. The Unit has undertaken the translation, designing and formatting of print-ready copies of books which it has published in collaboration with different publishing houses for use by teachers and students to improve science education in schools and colleges. In addition, the Unit is actively involved in science popularisation programmes, teacher training workshops in science education and in the development of small scale kits to conduct simple, interesting science experiments with a view to modernise science teaching at various levels of education.
The end-users of the multimedia CD-ROM packages were identified as students in high schools and colleges. It was decided that the package would not be strictly based on any particular school curriculum. It would be supplementary material with the main objective of creating interest in various disciplines, with emphasis on experimental science. The CD-ROMs and books developed and produced at ETU are:

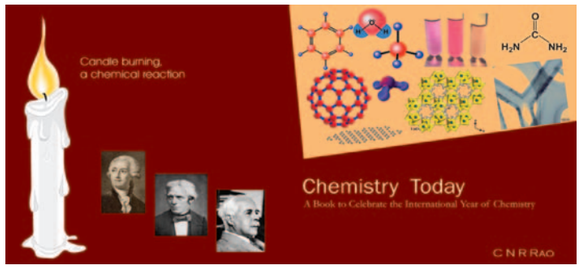
- UNDERSTANDING CHEMISTRY by Prof. CNR Rao (Book and CD-ROM)
- LEARNING SCIENCE by Prof. CNR Rao and Mrs. Indumati Rao (2 CD-ROMs and 4 Books)
- VIGNYANA KALIYONA (4 CD-ROMs and books in Kannada)
- VIGYAN SEEKHE (4 books in Hindi)
- BHUGOLA PARICHAYA (A CD-ROM in Kannada on geography)
- OUR EARTH IN THE SKY (A CD-ROM on astronomy)
- NANOWORLD by Prof. CNR Rao (An Introduction to Nanoscience and Technology) (Book and CD-ROM)
- CHEMISTRY TODAY (Books in English, Hindi and Kannada)
- RASAYAN VIGYAN KI DUNIYA (Book in Hindi)
- NANOPRAPANCHA (Book in Kannada)
- RASAAYANUSHAASTRADA ARIVU (Book in Kannada)

CNR Rao Hall of Science was inaugurated by the Hon. Prime Minister Dr. Manmohan Singh on December 3, 2008. It was established to have a dedicated venue for direct contact programmes to popularise Science among students and to enhance the skills of science teachers.

ETU is located at CNR Rao Hall of Science and is engaged in organising and participating in the various activities of CNR Rao Hall of Science.

CNR Rao Hall of Science and Education Technology Unit have organised and conducted Teacher-student programmes/ workshops as part of the Science Outreach programme. These programmes have been conducted in Physics, Chemistry and Biology at the Madan Mohan Malaviya Amphitheatre, CNR Rao Hall of Science, regularly from the time of its inception. In all these programmes, faculty from different institutes were invited to give lectures on a particular theme in the concerned subject and were also invited to participate in an interactive question-and-answer session at the end of the programme. Students and teachers from various schools and colleges in and around Bangalore, Bangalore Rural, Jawahar Navodaya Vidyalayas (Southern Region) and from different parts of Karnataka have attended these programmes. In each of these programmes atleast 200-225 students and teachers have participated.

The book titled `Chemistry Today', authored by Prof. CNR Rao to celebrate the International Year of Chemistry (IYC-2011) was formatted and produced by ETU. This was released at a function organised by the Chemical Research Society of India in association with Division of Chemical Sciences, IISc on January 1, 2011 by Prof. CNR Rao at the JN Tata Auditorium to inaugurate 'The International Year of Chemistry'. The book was distributed to all the participants.

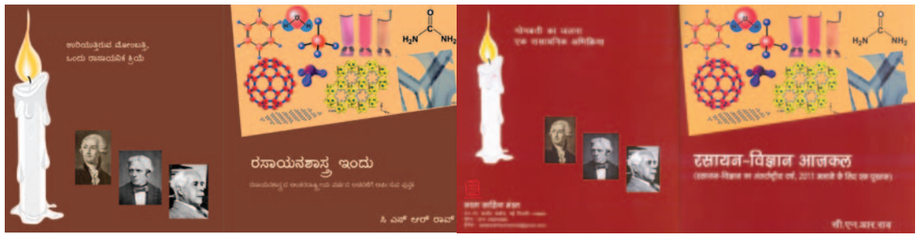


In celebration of the International Year of Chemistry, IYC-2011, the CNR Rao Hall of Science and ETU organised and conducted several programmes in Chemistry for students and teachers (some in association with other Units and institutions).

Programme for students (IYC-2011) (Jointly organised by ETU and NCU, JNCASR)	11 January 2011
'Chemistry in our lives' (IYC-2011)	24 February 2011
Special programme for students and teachers in Chemistry	14 June 2011
Chemistry for students and teachers (Jointly organised with Oracle Education Foundation as part of IYC-2011 programme)	27 July 2011
Chemistry programme - IYC -2011	7 December 2011

ETU completed the Hindi translation of `Chemistry Today' and both the English and Hindi versions of `Chemistry Today' are published and marketed by M/s Sastha Sahitya Mandal, New Delhi.

The book titled `Chemistry Today' was translated into Kannada by Mrs. Indumati Rao and formatted and completed for printing by ETU for Karnataka Rajya Vignyana Parishat for distribution to schools and colleges in Karnataka.



CNR Rao Hall of Science and Education Technology Unit along with SOP-ETU took up a project sponsored by the Vision Group on Science & Technology, DST, Govt. of Karnataka to conduct four workshops for 100 Pre-University Teachers from different places in Karnataka in using the College Chemistry Kit. The project involved assembling 200 numbers of College Chemistry Kits. The kit consists of 32 plastic/glass laboratory items, 85 solid and liquid chemicals for carrying out chemistry experiments.

The aim of the above workshops was to enable teachers to carry out experiments using very small quantities of the chemicals very effectively and safely even in the absence of a regular laboratory. ETU took the responsibility of designing, printing and labeling the various chemicals, labware, etc in the kit, procurring the chemicals and the labware required for the kit and the assembly of the kits. Four two-day workshops were conducted in batches of 25 teachers by SOP-ETU on April 1-2, April 6-7, April 11-12 and April 15, 2011. At the end of each workshop, each teacher was presented with two Kits to take back to their colleges.

In the area of science popularization, `Nanoworld', `Learning Science' 'Celebration of Chemistry' and `Vignyana Kaliyona' (a science popularisation program in Kannada for the benefit of Kannada medium school children), programmes were conducted at different places in the country.

The science popularisation programme "Learning Science" was organised at Pithoragarh, Uttarakhand in association with JB Memorial Manas Academy and sponsored by CNR Rao Education Foundation on May 18, 2011. Prof. CNR Rao gave the theme lecture followed by a 30-minute multimedia presentation by Mrs. Indumati Rao. This presentation consisted of excerpts from the Hindi CD-ROM titled `RasayanVigyan Samaje' (Understanding Chemistry in Hindi) developed and produced by Education Technology Unit, JNCASR. Around 250 students attended the programme. RasayanVigyan Samaje CD-ROMs and Learning Science books were distributed to the teachers attending the program.

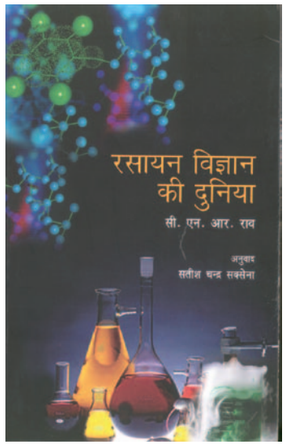
On June 30, 2011, CNR Rao Hall of Science and ETU organised and conducted the programme to award the prizes to Outstanding Science Teachers for the year 2010, donated by the CNR Rao Education Foundation, followed by a lecture programme. Prof. CNR Rao gave the lecture titled `New dimensions of Chemical Science'. Shri. Arvind Gupta gave the talk `Science through activities' along with demonstrations. This was followed in the afternoon by a lecture `The World of the Elephant' by Prof. R Sukumar. About 200 students and teachers participated in the programme.

The programmes organised and conducted by the CNR Rao Hall of Science and ETU in addition to the IYC programmes mentioned above are:

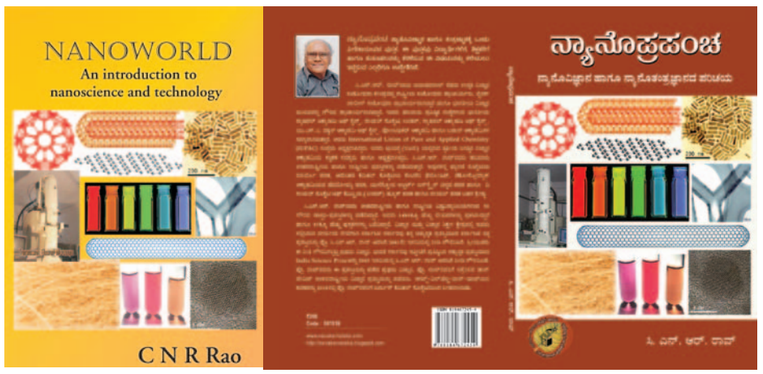
Programme for Engineering Sciences	24 January 2011
INSPIRE PROGRAMME	9 March 2011
Biology for students and teachers	5 August 2011
Physics for students and teachers	23 September 2011
Biology for students and teachers	14 October 2011
Physics for students and teachers	24 November 2011
INSPIRE PROGRAMME	29 December 2011

All the above programmes were conducted at the Madan Mohan Malaviya Amphitheater, CNR Rao Hall of Science, JNCASR.

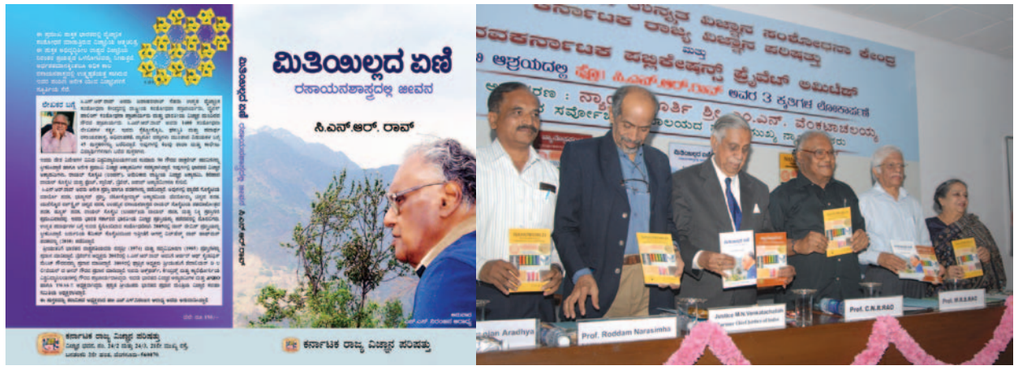
National Book Trust has published the first edition of the Hindi version of the Book 'Understanding Chemistry' titled `RasayanVigyan ki Duniya' in 2011.



The book Nanoworld: An Introduction to Nanoscience and Technology, authored by Prof. CNR Rao was translated by Mrs. Indumati Rao. The book was edited, formatted and made print-ready by ETU for NavaKarnataka Publications Ltd.



NavaKarnataka Publications Ltd. has published the book `Nanoworld' (in English) and the Kannada version – Nanoprapancha. The books were released at a function held at JNCASR on 24 October, 2011.



Prof. CNR Rao's autobiography `Climbing the limitless ladder' was translated into Kannada and edited by Mrs. Indumati Rao for the Karnataka Rajya Vijnana Parishath which has published the book. It was released at a function held on October 24, 2011 at JNCASR.

The Book `Understanding Chemistry' was translated into Kannada by Mrs. Indumati Rao. It was edited, formatted and completed for printing by ETU for Karnataka Rajya Vijnana Parishath.

The CNR Rao Hall of Science and Education Technology Unit will be organising workshops and programmes for teachers and students in different subjects like Physics, Chemistry, Biology, and Nanoscience as part of the Science Outreach programme. It is proposed to have lectures and demonstrations with different themes in a particular subject.

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PROFESSOR

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KR Sreenivasan

ENGINEERING MECHANICS UNIT

The Engineering Mechanics Unit pursues research on a variety of topics where fluid and heat transfer play a critical role in providing insight into various phenomena. Research work done in the Unit has relevance in many technological applications and variety of phenomena encountered in nature.

Research on dynamics of suspensions, bubbly and granular flows explore fundamental-problems, and their applications in chemical and other technologies. Research on granular matter in the Unit has helped in understanding the origin of shear-banding instabilities and resulted in showing that the vorticity banding can appear both as first-order and second-order phase transitions. Research work on suspension include, analysis on the orientation-dynamics of spheroidal particles in shearing flows, effects of inertia on the non-Newtonian rheology of a dilute emulsion, evolution of sedimenting particle clouds, and stability of fibrous suspensions at finite Reynolds number. Research on this topic has helped in identifying a new mechanism for the instability in a dilute suspension of active particles.

Biological problems - swimming of micro-organisms & flight of insects - are being investigated employing both theoretical and experimental methods. Research on unsteady aerodynamics of insect flight involving experiments and simulations using discrete vortex method, has helped in identifying new-mechanism of lift generation and its enhancement by controlled wing-flexibility, this work is relevant to the design of micro air vehicles.

Work is in progress on entropic lattice Boltzmann method, to study a variety of fluid flow problems, including turbulence, polymeric fluid and suspensions. A solver has also been developed for flutter prediction in turbo-machines.

Research relevant to geophysical processes include modeling mantle convection, cloud dynamics and nocturnal atmospheric boundary layer. These problems are being investigated through experiments and numerical simulations. Since clouds exhibit unusual characteristics in entrainment of ambient air, current research in the Unit explores this interesting phenomenon. Research in the Unit, on the study of nocturnal atmospheric surface-layer, has helped in identifying an error in radiation-codes widely used by atmospheric community and in solving an eighty-year old micro-metrological mystery- formation of the Ramdas-layer. Experiments done in the Unit, demonstrate the importance of aerosols in shaping temperature profile and the energy-budget of the nocturnal atmospheric surface-layer.

The Unit's faculty members are engaged in extensive collaborations with scientists located elsewhere in India and abroad. Examples of recent collaborations within India have been with the National Aerospace Laboratories (NAL) and IISc Bangalore; international collaborations include those with, Intel, Computational Research Lab (Pune), Boeing Research Centre (USA), University of Twente (The Netherlands) and Max-Planck Institute for Marine Microbiology (Bremen, Germany). External funding agencies supporting research-projects in EMU include BARC-Mumbai, DRDO, DST, NPOL Kochin and US-AOARD, Japan.

RECENT THESES (2011-2012)

- Kinetic theory and burnett order constitutive relations for a smooth granular gas [Vinay Kumar Gupta, MS(Engg), 2011]
- Vortex shedding patterns, their competition, and chaos in flow past inline oscillating rectangular cylinders [Srikanth T, MS(Engg), 2011]
- Experiments on vibrated granular materials: waves, convections and segregation [Mohammed Istafaul Haque Ansari, MS(Engg), 2012]
- Statics and dynamics of drops on solid surfaces: theory and simulations [Sumesh P T, Ph.D., 2012]

Meheboob Alam

MEHEBOOB ALAM RECEIVED HIS Ph.D. FROM THE INDIAN INSTITUTE OF SCIENCE. HE IS A RECIPIENT OF THE ALEXANDER VON HUMBOLDT FELLOWSHIP AND THE INAUGURAL RECIPIENT OF THE ASIAN YOUNG FLUID DYNAMICIST AWARD.

GRANULAR MATTER AND OTHER COMPLEX FLUIDS

Granular materials, a collection of macroscopic particles, are important in chemical processing and pharmaceutical industries, as well as in geophysical contexts, such as avalanches, volcanic eruptions, and sand dunes. Flowing granular materials belong to the class of complex, i.e., rheologically complex, fluids. Typical examples of complex fluids include suspensions, polymers, and worm-like micelles. In my Group, we carry out particle-level simulations, formulate rheological models, and analyse continuum models of granular matter and other complex fluids, with a goal to improve current mathematical models.

INSTABILITIES, PATTERNS, RHEOLOGY AND SEGREGATION

We have developed the Landau-Ginzburg order-parameter theory for the shear-banding phenomenon and other spatio-temporal patterns in a sheared granular fluid. Our linear stability theory has successfully predicted the onset of convection in a granular Rayleigh-Benard set up, and the related nonlinear theory has recently been developed. We have started a concerted effort to probe non-Newtonian and micropolar rheology, non-Gaussian velocity fluctuations and jamming transition in granular matter. In a project related to granular segregation, we have recently proposed a unified model explaining reverse buoyancy and non-monotonic ascension dynamics of Brazil nuts.

GEOPHYSICAL FLOWS

In the context of large Prandtl number convective flows, which are important in many geophysical contexts like magma, and mantle plumes, we have discovered a new buoyancy-driven instability mode in a plane thermal plume. Our current focus is to investigate the nonlinear stability and related mixed convection phenomena with non-Boussinesq approximation. We have also initiated theoretical work on porous media flows, focussing on volume averaged equations, interfacial/ boundary conditions and pattern formation.

EXPERIMENTAL FACILITY

On the experimental front, we have recently procured a “volumetric” Particle Image Velocimetry (v-PIV) system, the first of its kind in India, to measure three-dimensional unsteady velocity field in mixing of different fluids as well as in granular flows and suspensions. Experiments on shaken granular matter have been initiated, with a focus to uncover pattern formation scenarios and segregation mechanisms.

KEY PUBLICATIONS

P Shukla, and M Alam, *Weakly nonlinear theory of shear-banding in granular plane Couette flow,* **Journal of Fluid Mechanics 666,** 204 (2011).

KC Smith, T Fisher, and M Alam, *Isostaticity of constraints in amorphous jammed systems of soft frictionless Platonic solids,* **Physical Review E (Rapid Comm) 84,** 030301 (2011).

M Alam, and V Chikkadi, *Velocity distribution function and correlation in granular Poiseuille flow,* **Journal of Fluid Mechanics 653,** 175 (2010).

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Deepthi S

Santosh Ansumali

SANTOSH ANSUMALI RECEIVED HIS Ph.D. IN MATERIAL SCIENCE AT ETH, ZURICH, AND WAS A POST-DOCTORAL FELLOW IN ENERGY TECHNOLOGY THERE. HE WAS AN ASSISTANT PROFESSOR AT NANYANG TECHNOLOGICAL UNIVERSITY, SINGAPORE BEFORE JOINING JNCASR IN 2009. HE HAS RECEIVED THE ETH GOLD MEDAL FOR HIS Ph.D. THESIS, AND IS A RAMANUJAN FELLOW.

MESOSCALE SIMULATIONS AND HIGH PERFORMANCE COMPUTING

MESOSCALE SIMULATION ALGORITHMS

The creation of simplified minimal molecular dynamics for realistic applications has emerged as an important branch of modern computational statistical physics. The ultimate goal is to create Minimal Molecular Dynamics: small, but realistic, models of fluid flows. In such modelling approaches, the basic idea is that the same macroscopic dynamics can result from the collective motion of different underlying microscopic dynamics.

In the last decade, mesoscale algorithms such as Lattice Boltzmann models (LBM) or Dissipative Particle Dynamics (DPD) have highlighted the advantage of such approaches. For example, instead of continuum models such as the incompressible Navier-Stokes equation, LBM is now routinely used for computer simulations of fluid flows.

In our lab, we work on algorithmic development as well as applications of such tools for a variety of applications, ranging from incompressible hydrodynamics, to gaseous microflow, and rheology.

KINETIC SCHEMES FOR FOKKER-PLANCK EQUATION

The Fokker-Planck equation appears very often in the modeling of complex fluid as well as in other branches of physics and economics. So far, most of the popular methods to solve Fokker-Planck equation rely on link with equivalent Langevin equation which leads to a stochastic solver via Brownian dynamics. A direct solver is desirable from the point of view of possible increase in speed from deterministic formulation. We have formulated a solver of Fokker-Planck based on relaxation approximation.

HIGH PERFORMANCE COMPUTING

We are developing expertise both in terms of algorithm developments as well as creating high end codes which can be used by engineering community at large. In this regards, we have developed high performance code using Lattice Boltzmann for hydrodynamics, rheology, etc. Furthermore, we have developed a DNS code for exploring high-resolution transient flows.

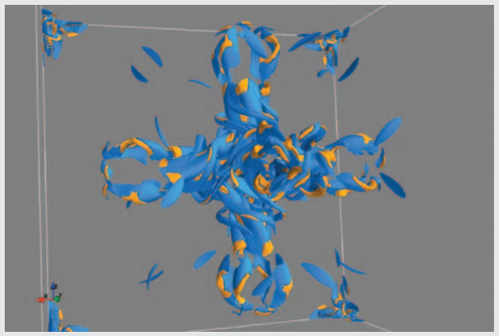
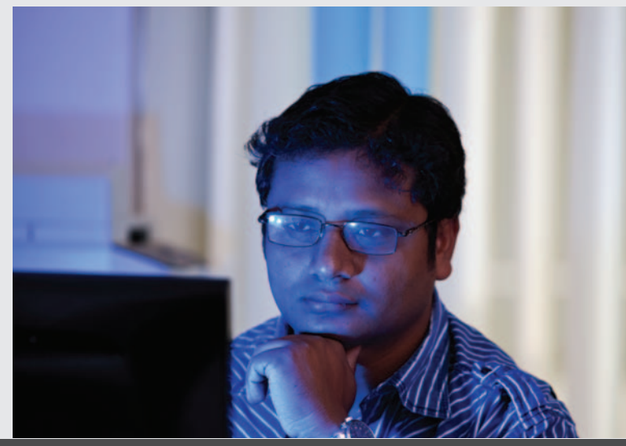


Fig. : Vortex Dynamics in High Reynolds number Kida Flow



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Rama Govindarajan

RAMA GOVINDARAJAN RECEIVED HER Ph.D. IN AEROSPACE ENGINEERING FROM THE INDIAN INSTITUTE OF SCIENCE, BANGALORE. SHE DID HER POST-DOCTORAL RESEARCH AT THE CALIFORNIA INSTITUTE OF TECHNOLOGY, AND WAS AT THE NATIONAL AEROSPACE LABS BEFORE JOINING JNCASR IN 1998.

INSTABILITIES AND INTERFACIAL FLOWS

For Newtonian fluids in relatively simple geometries, laminar flow is well-studied, both, experimentally, and theoretically. We know a lot about the statistical characteristics of homogeneous isotropic turbulence, but not so much about the turbulence in shear flows that occur all around us. What we understand the least is what makes a certain laminar flow become turbulent, and also what the route for completing the transition is. Instability and transition to turbulence is a focus area of this Group. Since the main interest is in flows where properties change across the flow, potential applications are in atmospheric, ocean and chemical engineering flows.

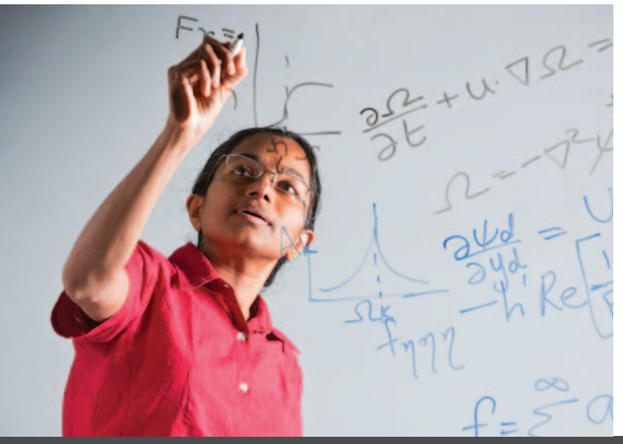
This Group is also interested in looking into the physics of interfacial flows like film flow and droplet evolution, where surface tension plays a major role. A description of ongoing exploratory work, in many areas where we don't have answers yet, is given below:

Sumesh PT is working on the dynamics of liquid drops in the presence of gravity and Marangoni stresses. He has shown how an infinitely long pendant drop with many lobes can exist in theory. He has also shown that when a liquid drop sits on a solid plate inclined to the horizontal, the plate can partly aid and partly oppose gravity. The dynamics are simulated by a lattice Boltzmann algorithm.
Collaborators: Ronojoy Adhikari, Ignacio Pagonabarraga

Croor Singh is interested in clouds -- scientifically, and poetically. He is beginning to understand how a cloud is formed, and how long it lives.
Collaborator: R Narasimha

Sharath Jose, along with Anubhab Roy, is trying to understand disturbance evolution in channel flows, across which viscosity and gravity vary.
Collaborators: Luca Brandt, Dan Henningson

Mamta Jotkar wishes to know how wall geometry affects the transition to turbulence in the case of channel and pipe flows, and how we may control it.
Collaborators: VassilisTheofilis, Gayathri Swaminathan, Kirti Sahu



Rohith VS and Deepak Rao are trying to understand vortex merger.

Divya Venkataraman has had fun results with a "hairfoil", an airfoil with long cilia (hair) stuck on it computationally. She has shown that drag and lift are modified considerably by the cilia, and is trying to explain why.
Collaborator: Alex Bottaro

Debasish Saha is interested in the flow of complex fluids like laponite, a designer clay. He is studying how this substance ages, i.e., how its viscosity changes with time.
Main Advisor: Ranjini Bandyopadhyay

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MS STUDENT
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Roddam Narasimha

R NARASIMHA DID HIS BE AT UVCE, AND MASTER'S (BY RESEARCH) AT IISC, BANGALORE. HE RECEIVED HIS Ph.D. IN AERONAUTICS AND PHYSICS FROM THE CALIFORNIA INSTITUTE OF TECHNOLOGY.

AEROSPACE AND ATMOSPHERIC FLUID MECHANICS

My major interests have been in the fluid dynamics associated with aerospace and atmospheric sciences. A connecting link between the two is that of turbulent fluid flow, which plays an important role in both fields.

In aerospace problems, recent interest has focused on the design of optimal wing planforms for propeller-driven aircraft that enhance the inherently greener characteristics of the propeller compared to turbojet or fan engines. The optimal designs involve novel planforms, and have recently been computed for a wide variety of practical constraints. International patents based on this work have recently been filed.

In atmospheric science we have successfully simulated the form, evolution, and entrainment characteristics of natural clouds in the laboratory. This work indicates that a suitable low-order fluid dynamical model for the cumulus cloud is a transient diabatic plume. Off-source heat release in such a plume constitutes a crucial link between microphysics and fluid dynamics in a cumulus cloud. Accurate measurements of the entrainment rates are now being made in the laboratory.

Extensive studies have been made of the development of a turbulent mixing layer in a point vortex gas. These simulations show that such mixing layers have ultra-long memories of initial conditions, but that in the asymptotic limit, the rate of growth of the thickness of the layer is independent of the initial conditions.

KEY PUBLICATIONS

R Narasimha, SS Diwan, S Duvvuri, KR Sreenivas, and GS Bhat, *Laboratory simulations show diabatic heating drives cumulus-cloud evolution and entrainment,* **PNAS 108,** 16164-16169 (2011).

BR Rakshith, SM Deshpande, C Praveen, and R Narasimha, *Assessment of lifting-line theory optimization of turboprop wings in tractor configuration using Euler code,* **Proc. Symp. Applied Aerodynamics and Design of Aerospace Vehicles,** 564 (2011).

R Narasimha, *Satish Dhawan,* **in: A Voyage Through Turbulence (ed. P Davidson et al.),** Cambridge University Press (2011).

S Suryananrayana, and R Narasimha, *Point-Vortex Simulations Reveal Universality Class in Growth of 2D Turbulent Mixing Layers,* **arXiv:1008,** 2876v1 [physics.flu-dyn] (2010).

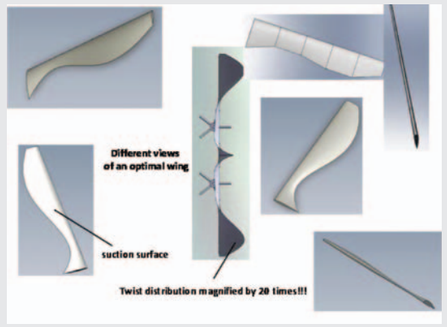
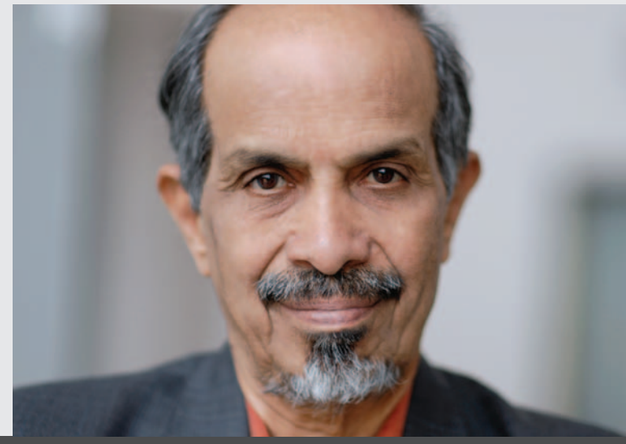


Fig. : Novel optimal wings for turboprop aircraft viewed from different angles. One in the middle is seen from behind the wing; two at the right are edge-on views, looking at the leading edge



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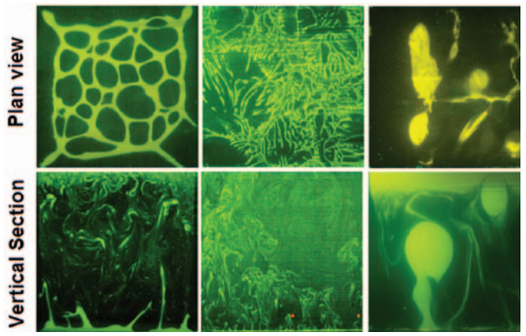
KR SREENIVAS RECEIVED HIS Ph.D. FROM THE INDIAN INSTITUTE OF SCIENCE, BANGALORE. HE WAS AT THE UNIVERSITY OF DELAWARE, NEWARK, DELAWARE, AS A POST-DOCTORAL RESEARCH FELLOW BEFORE JOINING JNCASR.

FLUID MECHANICS AND HEAT TRANSFER

Our Group is currently working on the unsteady aerodynamics of insect flight, the role of radiative heat transfer in the nocturnal atmospheric surface layer, double-diffusive finger-convection, the dynamics of hydraulic jumps, microphysics of cloud development, and natural ventilation using cooling towers, earthen-tunnels and other methods.

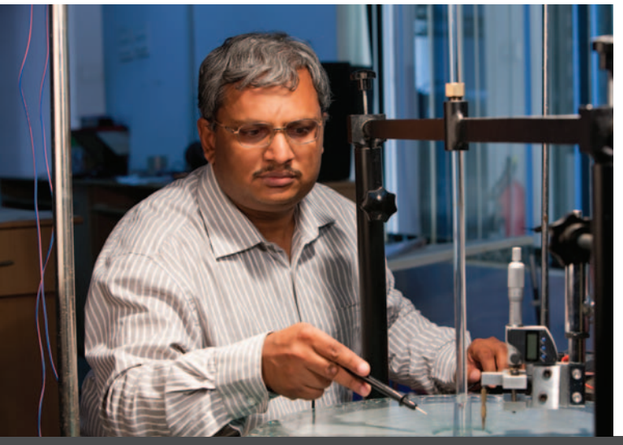
CONVECTION IN THE LIMIT OF HIGH RAYLEIGH AND PRANDTL NUMBERS

Mantle convection is responsible for volcanism and plate-tectonics. Laboratory modelling of the mantle convection is extremely challenging. We experimentally simulate convection in the limit of large Rayleigh number by using concentration differences. Experiments are done in a regime corresponding to a high Prandtl number limit, & with viscosity difference between plume fluid and the ambient medium. These experiments capture some aspects of mantle convection (Figure 1, convection patterns with varying viscosity contrast).



LIFTED TEMPERATURE MINIMUM (RAMDAS LAYER)

On calm and clear nights, the minimum in the vertical temperature profile occurs a few decimeters above the ground and is known as Lifted temperature minimum (LTM). Work on this area in our group has resulted in identifying an error in the flux-emmisivity model for radiation used by many researchers in the atmospheric community. The error was responsible for spurious cooling reported in many studies; its effect extended all the way up to 1km in the boundary layer and showed unrealistic sensitivity to the ground emissivity. Related experimental work (both in laboratory and field) has helped in explaining formation of LTM, which was an eighty years old micro-meteorological mystery. We identified that atmospheric aerosols are primarily responsible for this phenomenon and results have impact on the prediction of radiation-fog, and in prescribing the sensible-heat boundary condition for weather and climatic models.



UNSTEADY AERODYNAMICS OF INSECT FLIGHT

Research in the area of flapping flight has attracted renewed interest due to its possible application in Micro Air Vehicles (MAVs). For a sustained and high endurance flight, with a larger payload-carrying capacity, we need to identify a simple and efficient flapping-kinematics. Our experiments and discrete vortex method (DVM) simulations have shown that a simple asymmetric-flapping could generate sustained lift. Our results also indicate that for a given flapping amplitude, the lift generated can be maximized by choosing optimum wing inclination and wing-flexibility.

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GANESH SUBRAMANIAN HAS A Ph.D. (2002) IN CHEMICAL ENGINEERING FROM THE CALIFORNIA INSTITUTE OF TECHNOLOGY, USA. HE WAS A POST-DOC AT CORNELL UNIVERSITY, USA, BEFORE JOINING JNCASR IN NOVEMBER 2005.

RHEOLOGY OF COMPLEX FLUIDS, VORTEX DYNAMICS, TRANSPORT PROCESSES IN THE NOCTURNAL BOUNDARY LAYER

A major theme relates to modeling transport processes in complex fluids. Topics of interest include the orientation dynamics of anisotropic particles in shearing flows, evolution of sedimenting particulate clusters, and fluid dynamics of microbial suspensions.

Our research on vortex column oscillations has revealed the continuous spectrum of an inviscid vortex column. These singular oscillations underlie its response to ambient turbulence, and lead to a modal representation for an evolving vortical disturbance. The analysis relates the modal and non-modal approaches to hydrodynamic stability.

The subtle role of radiation in the Nocturnal Boundary Layer (NBL) is highlighted by the Lifted Temperature Minimum (LTM) phenomenon that involves a preferential cooling of the near-surface air layers on calm clear nights. The prevailing explanation for the LTM is erroneous: the latter requires a heterogeneous atmosphere, with the near-surface aerosol concentration gradient being responsible for this heterogeneity. The error affects a wide class of models, and, to this end, we have provided the correct formulation governing radiative interactions between reflective surfaces.

KEY PUBLICATIONS

DL Koch, and G Subramanian, *Collective hydrodynamics of swimming micro-organisms: Living fluids,* **Annual Reviews of Fluid Mechanics 43,** 637-659 (2011).

G Subramanian, DL Koch, and Sean R Fitzgibbon, *The stability of a homogeneous suspension of chemotactic bacteria,* **Physics of Fluids 23,** 41901 (2011).

G Subramanian, and DL Koch, *The influence of the inertially dominated outer region on the rheology of a dilute suspension of low-Reynolds-number drops and particles,* **Journal of Fluid Mechanics 674,** 307-358 (2011).

Ganesh Subramanian, *Viscosity-enhanced bio-mixing of the oceans,* **Current Science 98(8),** 1103-1108 (2010).

V Mukund, VK Ponnulakshmi, KS Dheeraj, G Subramanian, and KR Sreenivas, *Hyper-cooling in the nocturnal boundary layer: the Ramdas paradox,* **Physica Scripta T142,** 14041 (2010).

Vivek R Raja, G Subramanian, and DL Koch, *Inertial effects on the rheology of a dilute emulsion,* **Journal of Fluid Mechanics 646,** 255-296 (2010).

G Subramanian, *Wading through Batchelor's book,* **Resonance Journal of Science Education 15(4),** 363-383 (2010).

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FACULTY FELLOW

Kavita Jain*

*Jointly with TSU

EVOLUTIONARY AND ORGANISMAL BIOLOGY UNIT

Biological systems are organised in a hierarchical manner structurally, and can be studied at levels ranging from molecules to ecosystems. Decades of narrowly focussed studies at one or the other level of structural complexity have greatly enhanced the body of information we possess about biological systems, leading to a state exemplified by TS Eliot's lament: "Where is the knowledge we have lost in information?" Consequently, biology today is at an integrative phase, in which we are attempting to synthesize vast amounts of information into a holistic understanding of how living systems function and evolve.

Although biological systems are hierarchical in terms of structure, functionality in biological systems is typically integrated across scales of structural complexity. Functionality in biological systems, moreover, needs to be interpreted and understood in a meaningful natural context. In the vast majority of cases, the principal structural level of complexity which is also a functionally integrated entity is the multicellular organism, and it is also the organism that is most often the primary unit upon which natural selection acts to shape the functionality of organisms over generations. Biological questions regarding the fundamental processes of life are, consequently, best posed in the context of an organism embedded in its ecology.

In Organismal Biology, the organism is the entity around which (a) questions regarding functionality in biological systems are framed, and (b) information gleaned from studies at various structural levels of biological complexity is welded together in an attempt to answer such questions. Actually, the term "Organismal Biology" is overkill: by and large, only organisms have a biology. Molecules do not have a biology any more than mathematical models do. Nevertheless, understanding the structure and dynamics of molecules, and of mathematical models, can be very useful in understanding the biology of organisms. Indeed, in its quest to understand functionality in living systems, Organismal Biology uses tools, techniques and information from a variety of disciplines, including molecular genetics, evolutionary genetics, biochemistry, physiology, neurobiology, behaviour, ecology, computation, physics, statistics, and mathematics.

Our Unit is one of the principal centres in the country for research and training in chronobiology, evolutionary genetics, population ecology, behavioural neurobiology, behavioural ecology and phylogeography. We do mostly empirical research, both in the lab and in the field, using a combination of experimental tools from evolutionary quantitative genetics, molecular genetics, neurobiology, developmental biology, animal behaviour, and population biology. We also conduct theoretical research, largely through computer simulations of mathematical models of biological processes. Our Unit is well equipped for studies using a range of experimental and computational tools, with labs for routine handling of large numbers of *Drosophila* populations, labs for experiments in physiology, biochemistry, molecular biology, genomics and immunocytochemistry, and three separate sets of Chronocubicles for maintaining *Drosophila*, ants and mice, under controlled light conditions, and monitoring various rhythms in these organisms. With over 6,500 channels, our activity recording system for insects and small mammals is the largest such facility in the world. The Unit also maintains a field station in HD Kote Taluk, Karnataka, for facilitating research in wildlife biology.

RECENT THESES (2011-2012)

- Role of social interactions in modulating circadian clocks in Camponotus ants and *Drosophila melanogaster* (Shahnaz Rahman Lone, Ph.D., 2011)
- Coherence, dynamics and stability in spatially structured and unstructured populations: effects of dispersal and crowding (Snigdhadip Dey, Ph.D., 2011)
- Behavioral and genetic analyses of fruit fly *Drosophila melanogaster* populations selected for morning and evening adult emergence (Koustubh M Vaze, Ph.D., 2012)
- Large and small ventral lateral neurons play vital roles in circadian and arousal circuits in *Drosophila melanogaster* (Sheetal Potdar, M.S., 2012)
- Evolution of precise circadian rhythms in fruit fly *Drosphila melanogaster* populations selected for adult emergence in a narrow window of time (Nisha N Kannan, Ph.D., 2012)

CITATION/AWARDS

2012: Prof Vijay Kumar Sharma elected Fellow of Indian Academy of Sciences

CITATION/AWARDS

2011: Prof Amitabh Joshi received Lakshmipat Singhania – IIM Lucknow Young Leader in Science & Technology Award

Vijay Kumar Sharma

VIJAY KUMAR SHARMA DID HIS PHD IN BIOPHYSICS AT THE NORTH EASTERN HILL UNIVERSITY, SHILLONG, AND WAS A GUEST RESEARCHER AT NTNU, NORWAY, BEFORE JOINING JNC AS FELLOW IN 1998.

CIRCADIAN RHYTHMS IN FRUIT FLIES AND ANTS

In our laboratory, we take an integrated approach to understanding circadian time-keeping mechanisms, using behavioural, evolutionary, sociobiological, physiological, and molecular genetic studies, augmented by manipulations of genes that modify circadian phenotype. Most of our work stems from laboratory selection paradigms using fruit fly populations. We carry out behavioural and molecular studies on *Drosophila* populations selected for different circadian phenotypes. In addition, we study the circadian rhythms of fruit flies under laboratory and semi-natural conditions, and examine the roles of genes previously implicated in circadian function.

Our work on the circadian rhythms of fruit flies and ants has provided the first ever empirical evidence for:
(a) evolution of circadian clocks through laboratory selection,
(b) adaptive significance of circadian clocks,
(c) carpenter *Camponotus* ants using circadian plasticity to manage challenges arising due to division of labor,
(d) independence of known clock genes and neurons in circadian timing system regulating egg-laying rhythm,
(e) evolution of precise circadian clocks as a result of selection on the timing of adult emergence,
(f) *Or47b* olfactory receptor neurons involvement in the regulation of nocturnal sex drive, and
(g) socio-sexual interactions causing long lasting after-effects in the circadian clocks of fruit flies and ants.

In a series of recent studies, we are looking at:
(i) neurogenetic bases of circadian egg laying rhythm in *Drosophila,*
(ii) molecular genetics of "morning" and "evening" circadian phenotypes in *Drosophila,* and (iii) circadian rhythms of fruit flies under semi-natural conditions.

KEY PUBLICATIONS

SR Lone, and VK Sharma, *Or47b receptor neurons mediate socio-sexual interactions in fruit flies Drosophila melanogaster,* **Journal of Biological Rhythms 27,**107-116 (2012).

NK Nisha, R Reveendran, S Hari Dass, T Manjunatha, and VK Sharma, *Temperature can entrain egg-laying rhythm of Drosophila but may not be a stronger zeitgeber than light,* **Journal of Insect Physiology 58,** 245-255 (2012).

SR Lone, and VK Sharma, *Timekeeping through social contacts: Social synchronization of circadian locomotor activity rhythm in the carpenter ant Camponotus paria,* **Chronobiology International 28,** 862-872 (2011).

SR Lone, and VK Sharma, *Social synchronization of circadian locomotor activity rhythm in fruit flies Drosophila melanogaster,* **Journal of Experimental Biology 214,** 3742-3750 (2011).

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Amitabh Joshi

AMITABH JOSHI RECEIVED HIS Ph.D. IN EVOLUTIONARY GENETICS FROM WASHINGTON STATE UNIVERSITY, AND PURSUED POST-DOCTORAL WORK AT THE UNIVERSITY OF CALIFORNIA, IRVINE. HE HAS ALSO BEEN FELLOW AT THE INSTITUTE OF ADVANCED STUDIES, BERLIN.

EVOLUTIONARY GENETICS AND POPULATION ECOLOGY

My principal interest is in trying to better appreciate and understand adaptive evolution as a dynamic process in which the interaction of the ecology and genetics of a population shapes its evolution. I am also interested in understanding the dynamics of population size, especially in spatially structured populations. Most of my research is empirical and laboratory based, using fruitflies (*Drosophila* spp) as a model system. I occasionally do theory too, but my theoretical work is very strongly motivated by and grounded in empirical studies. More recently, I have been intrigued by the possibility that the existing conceptual framework we have for describing and understanding evolution might have some serious shortcomings, and that new conceptual approaches may need to be developed to overcome them. This leads to a nascent but growing interest in many philosophical issues in evolution. I also have serious interests in poetry (urdu, english, and to a more limited extent farsi, braj, and punjabi), history, military science, philosophy, and many kinds of music, especially traditional qawwali.

My work on evolutionary genetics over the last decade has largely been built around selection experiments with *Drosophila.* Through selection, we have created populations with markedly reduced egg to adult development time. Comparison of the pre-adult traits evolved in these populations with those earlier seen to evolve in populations subjected to high larval crowding showed clearly that faster development and competitive ability are actually negatively correlated within populations, and comprehensively changed our understanding of the relationship between rapid development and competition in *Drosophila.* We are now using these populations to try and understand the genetic control of timing of key developmental events, as well as the developmental underpinnings of evolutionarily important variation in life-history related traits, an approach we have labelled developmental evolutionary biology or devo-evo. Other selection experiments are aimed at understanding the ways in which *Drosophila* adapt to extreme larval crowding, and the effects that such adaptations may have on population stability.

My research in population dynamics has been primarily focussed on understanding how life-history and environment affect the dynamics of population size in small populations and metapopulations. We showed theoretically that spatial variation in density could stabilize the behaviour of simple population models, providing a possible explanation for the ubiquity of stable dynamics in natural populations. We were the first to provide experimental validation of the hypothesis that population stability is likely to evolve as a by-product of life-history evolution through individual level natural selection acting on characters not directly related to population dynamics, and also the first to experimentally test hypotheses about the effects of migration on metapopulation dynamics and extinction patterns. We continue to study the impact of migration on metapopulation dynamics, both theoretically and experimentally.

KEY PUBLICATIONS

LD Mueller, and A Joshi, *Stability in Model Populations, Monographs in Population Biology 31,* **Princeton University Press,** Princeton, NJ, USA (2000).

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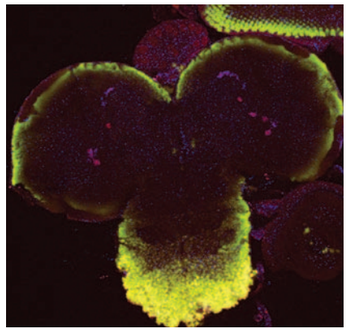
NEURONAL CIRCUITS IN FRUITFLIES

We study the ways in which neurons communicate with each other to regulate behaviours, using the fruit fly *Drosophila melanogaster*. Taking into account the wide variety of robust rhythmic behaviors that *Drosophila* exhibit, most of our studies focus on understanding the neuronal circuitry that regulates daily rhythms of activity, sleep, adult-emergence and egg-laying. We use an array of genetic tools available in flies to answer many of our questions.

In addition, we use the comparative approach to derive general models regarding how neuronal circuits function by examining other Drosophilid species such as *D. anannasae*, *D. malerkotliana*, *D. nasuta*, and *Zaprionus indianus*. Using a combination of behavioural, genetic, neuroanatomical, and molecular methods, we are also attempting to understand the possible role of temperature-sensitive ion channels such as the transient receptor potential channel, dTRPA1, in communicating with circadian clocks in *Drosophila*.

We also use the circadian neuronal circuit in fruit flies to model the progression of Huntington's disease – a neurodegenerative disorder – with the aim of understanding the links between behavioural defects and the underlying neuroanatomical and molecular dysfunction.



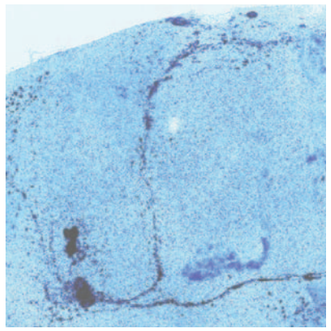


Fig. 1: Confocal image of larval brain of *D. melanogaster* expressing human Huntingtin protein (Red) in circadian neurons co-stained to reveal neurotransmitter PDF (blue) and pan-neuronal marker elav (green).

Fig. 2: Left hemisphere of adult *D. nasuta* brain stained with antibodies against neuropeptide PDF showing candidate circadian neurons and their projections. Confocal image re-rendered using Adobe photoshop.

KEY PUBLICATIONS

V Sheeba, KJ Fogle, and TC Holmes, *Persistence of morning anticipation behavior and high amplitude morning startle response following functional loss of small ventral lateral neurons in Drosophila*, **PLoS One 5(7),** e11628 (2010).

V Sheeba, *The Drosophila melanogaster circadian pacemaker circuit*, **J Genetics 87,** 485-493 (2008).

V Sheeba, KJ Fogle, M Kaneko, S Rashid, YT Chou, VK Sharma, and TC Holmes, *Large ventral lateral neurons modulate arousal and sleep in Drosophila*, **Current Biology 18,** 1537-1545 (2008).

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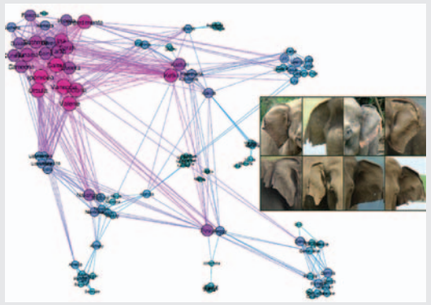
ANIMAL BEHAVIOUR AND SOCIOGENETICS

I am primarily interested in animal behaviour and sociogenetics, as well as phylogeography. The behaviour of social animals is a complex response to the physical environment, as well as to interactions with conspecifics, which may offer inclusive fitness benefits or may be a source of conflict. Understanding the relative roles of ecology and individual relationships in shaping animal societies is the motivation driving my present work. In my lab, we work on the social organization and behaviour of Asian elephants because they are socially advanced, inhabit diverse habitats, and offer opportunities for inclusive fitness benefits by living in family groups of related individuals. We try to a) understand the complexity of social organization in this species, which shows a fluid, fission-fusion society, not unlike that of humans, and b) find out how ecological factors and genetic relatedness between individuals influence associations, patterns of movement, and dominance relationships.

Our other project is on the comparative phylogeography of large mammals in the Western Ghats. This work arose from the intriguing discovery of a break in gene flow between elephant populations in the Western Ghats that were separated by the Palghat Gap. We are currently examining the population genetic structure and phylogeography of other large mammals with different generation times and dispersal abilities, in order to obtain insights into the biogeographic history of the Western Ghats.



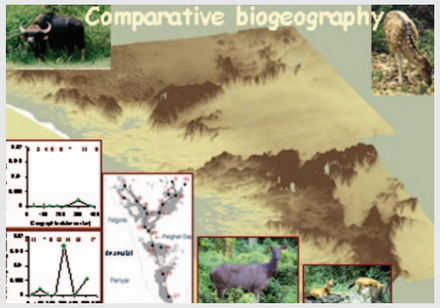


Fig. 1: (Image above) Some of the female elephants individually identified using ear characteristics (right) and the association network of identified adult female elephants (left)

Fig. 2: (Right side image) Comparative biogeography of large mammals in the Western Ghats. The panels on the left show the test for breaks in gene flow. There is no significant break in gene flow between elephants in an E-W direction (top panel) across the Nilgiris but a break in gene flow in the N-S direction (seen as a sharp peak in the bottom panel) corresponding to the Palghat Gap.

KEY PUBLICATIONS

Shetty NR, Vidya TNC, *To split or not to split: the case of the African elephant*, **Current Science 100:** 810-812 (2011).

Vidya TNC, Thuppil V, I*mmediate behavioural responses of humans and Asian elephants in the context of road traffic in southern India*, **Biological Conservation 143:** 1891-1900 (2010).

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K S Valdiya

KS VALDIYA IS AN INSA GOLDEN JUBILEE RESEARCH PROFESSOR

NEOTECTONICS AND ENVIRONMENTAL GEOLOGY

The identification of belts where sudden and swiftly occurring geological phenomena often destabilize the natural configuration of life, and threaten the balance of ecosystems, is the principal objective and the main thrust of activities of this one-man Unit. Regions vulnerable to landslides and occurrence of earthquakes repeatedly in the central sector of the Himalayan arc, including the Indo-Tibetan border region, Kumaun (Uttarakhand, Himalaya), the Biligirirangan Range in south-eastern Karnataka, the Sahyadri Range, and the coastal belt in western Karnataka and central Kerala were taken up for studies. Various signs of physical changes taking place in the natural systems in the study areas were interpreted through the analysis of patterns in topographical maps and satellite imagery, intensive as well as extensive field work, interpretation of uncommon behaviours of rivers and streams in response to continuing tectonic movements, and visual observations of common hazard indicators.

The field-based studies demonstrated that geomorphological rejuvenation of landforms, changes in courses of rivers, their anomalous knee bends, and their blockages manifesting itself in the formation of lakes, and subsequent development of flat ground of black clay deposits; modification of landform due to acceleration of gully erosion; and the development of mountain or hill barriers along active faults in south-eastern Karnataka and adjoining Tamil Nadu, the southern Sahyadri and its foothill belt in central Kerala, and in the Sor Valley in eastern Kumaun in Uttarakhand, Himalaya, are related to continuing movements on ancient faults. It is realized that the reactivation in the present time of older faults is contributing towards a relaxation of strain in the earth's crust in these earthquake-prone belts. Another area of study is the delineation of a regional terrane-defining boundary fault in the High Himalaya, gaining insight into the mechanism of recent movements on it, and obtaining information on the changes taking place.

The current activities include the writing of books in simple language for students, teachers and researchers in geology, as well as laymen, on the geodynamic history of the Indian continent, natural hazard mitigation, state of the natural environment of India, and the geodynamic events in the prehistoric periods of India. There is also a very active involvement in the Science Outreach Programme in remote regions of Uttarakhand, sponsored and funded by the CNR Rao Hall of Science.

KEY PUBLICATIONS

KS Valdiya, **Geology, Environment and Society,** Universities Press, Hyderabad (2004, 2011).

KS Valdiya, *Trans-Himadri fault: Tectonics of a detachment system in central sector of Himalaya,* **Jour. Geol. Soc. India 65,** 537-552 (2006).

KS Valdiya, **Saraswati: The River that Disappeared,** Universities Press, Hyderabad (2002).

KS Valdiya, **Himalaya: Emergence and Evolution,** Universities Press, Hyderabad (2001).

KS Valdiya, *Tectonic resurgence of the Mysore plateau and surround region in cratonic Southern India,* **Current Science 81,** 1068-1089 (2001).

KS Valdiya, **Dynamic Himalaya,** Universities Press, Hyderabad (1998).

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INTERNATIONAL CENTRE FOR MATERIALS SCIENCE

The International Centre for Materials Science (ICMS), at the Jawaharlal Nehru Centre for Advance Scientific Research, is devoted to carry out high impact interdisciplinary research, promote collaborations, personnel exchange, organize discussions and meetings and promote education in Advanced Materials Science. ICMS was dedicated to the nation by Prime Minister of India Dr. Manmohan Singh on December 03, 2008. The Centre is financially supported by the Department of Science and Technology (DST), Government of India and directed by Professor C.N.R. Rao, F.R.S.

The ongoing research programs are Chemistry of Materials, Surface physics Soft Condensed Matter and Low-dimension materials and other aspects of Materials Science. The Centre now houses several sophisticated research facilities such as molecular beam, epitaxy and other growth system, ultra high resolution TEM and state-of-the-art optical, electrical and magnetic characterization probes.
ICMS supports PhD and MS degree programmes, Short-term visits and offers Post-graduate Diploma in Materials Science.

The centre has established several collaborations and has signed Memorandum of Understanding with leading international research institutions such as Weizmann, SISSA, RMIT –Australia, Waterloo Canada, under which there are constant exchanges of students and researchers along with frequent technical meetings and workshops. The centre is a member of several International fora like EICOON, WMRIF and IUSSTF.

International Centre for Materials Science also conducts annual national and international lecture series by eminent scientists from all over the world. The fifth 'International Materials Science Lectures' was delivered by Prof. Chad A. Mirkin of Northwestern University, the 'Annual Materials Lecture' by Dr. Satishchandra B. Ogale, of CSIR-NCL and the 'Sheikh Saqr Materials Lecture' by Prof. J. M. D. Coey of Trinity College.

SHEIK SAQR LABORATORY

Of late, a Memorandum of Understanding with Ras al Khaimah Centre for Advanced Materials (RAK-CAM) was signed on December 3, 2011 between Prof. A. K. Cheetham, F.R.S., Chairman, Scientific Advisory Board of RAK-CAM and Prof. M.R.S. Rao, President, JNCASR. The support provided by RAK-CAM is being used to establish the Sheikh Saqr Laboratory (SSL) in ICMS and supporting various activities, lectures and Fellowships.

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THEMATIC UNIT OF EXCELLENCE ON COMPUTATIONAL MATERIALS SCIENCE

TUE-CMS

The Thematic Unit of Excellence on Computational Materials Science (TUE-CMS) is a project funded by the Nano Mission of the Department of Science and Technology. It was established in January 2012. This TUE continues and expands the activities carried out under the Centre for Computational Materials Science (CCMS) which was established in 2006. CCMS too was supported by the Nanoscience and Technology Initiative of DST. TUE-CMS operates under the International Centre for Materials Science at JNCASR.

Members of TUE-CMS carry out research in the broad area of computational materials science, using a variety of analytical and computational tools. They have strong interactions with groups engaged in experimental research in materials and biology. The list of topics studied in recent years is rich and diverse, including: the electronic structure of nanomaterials, charge transport and catalysis in nanosystems, novel magnetic materials and their properties, non-linear optical materials, multifunctional materials, spintronic materials, disordered systems, complex and molecular liquids, biomimetic systems and biomaterials. The techniques employed include ab initio calculations, molecular dynamics simulations, multiscale modelling and many body theory. Research is also carried out on developing various techniques and codes such as Monte Carlo simulations to predict gas adsorption isotherms in porous solids, enhancements in capabilities of first principles techniques and combined atomistic and contunnum methods to study meso-scale problems in materials. Around 50 original research articles are published by members of TUE-CMS every year.

The High Performance Computing Facility of TUE-CMS has two Infiniband based clusters, one containing 512 cores of Xeon Woodcrest processors with a theoretical peak rating of 6 TFLOPS and another of 400 cores of Xeon Nehalem processors. Augmentation of these facilities is currently ongoing. It is also envisaged to build a 1000 square feet modern datacentre as well as a hall with Virtual Reality Visualization capabilities.

Along with supporting the research programmes of its members, TUE-CMS carries out a number of outreach activities: in addition to an active Visitors' programme, several schools and conferences are conducted every year. The schools consist of theoretical and practical sessions. An Instructional Computing Laboratory, containing 30 computers enables the students attending workshops to acquire hands-on experience in writing and running sophisticated codes. Topics that have been covered in these schools include electronic structure methods, molecular simulations, numerical many-body methods in physics and chemistry, and biomolecular simulations. TUE-CMS is also committed to establishing international collaborations with institutions of equivalent high quality in the area of computational science.

www.jncasr.ac.in/ccms

Fig. 1 : Supercomputing facility

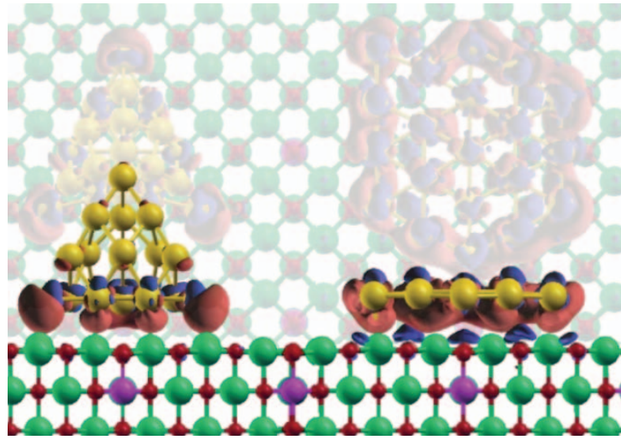

Fig. 2 : Doping the magnesia substrate with Al atoms triggers a change in the morphology of Au_{20} clusters on an MgO substrate {Mammen, Narasimhan and de Gironcoli, JACS, 133, 2801 (2011)}.

C N R Rao

CNR RAO, D.Sc. (MYSORE), Ph.D. (PURDUE), Sc.D. (HC), D.Sc. (HC), L.L.D. (HC), D.LITT. (HC), F.R.S., HON. F.R.S.C., HON. F. INST. P. IS A NATIONAL RESEARCH PROFESSOR, LINUS PAULING RESEARCH PROFESSOR AND FOUNDER AND HONORARY PRESIDENT OF JNCASR. HE IS ALSO THE DIRECTOR OF THE INTERNATIONAL CENTRE FOR MATERIALS SCIENCE (ICMS).

CHEMISTRY OF MATERIALS

RESEARCH INTERESTS

Oxide materials: Multiferroics, Electronic Phase Separations, Colossal Magnetoresistance (CMR)
Carbon Materials: Nanotubes and Graphene
Nanomaterials of all dimensionalities
Organic-inorganic hybrid materials including Kagome structures

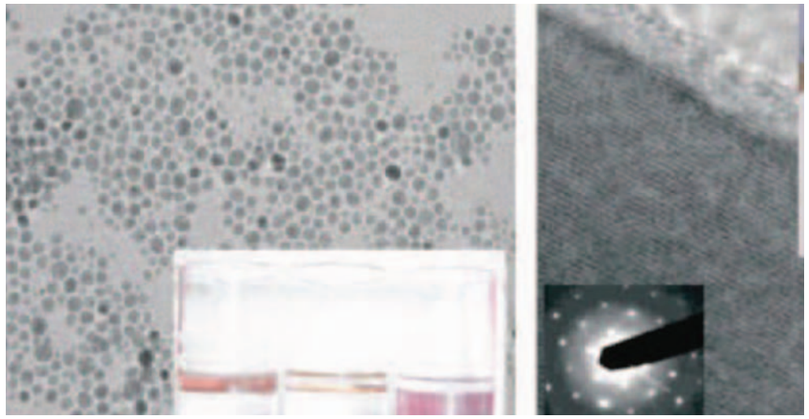

Fig. : Organic-water interface for large scale syntheses of nanocrystals and single crystalline films

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RANJAN DATTA OBTAINED HIS Ph.D. IN MATERIALS SCIENCE AND METALLURGY FROM THE UNIVERSITY OF CAMBRIDGE, UK. HE WORKED AS A POST-DOCTORAL RESEARCH SCIENTIST IN THE SCHOOL OF MATERIALS AT ARIZONA STATE UNIVERSITY BEFORE JOINING ICMS, JNCASR AS A FACULTY FELLOW IN 2008.

ABERRATION CORRECTED TRANSMISSION ELECTRON MICROSCOPY

ABERRATION-CORRECTED HIGH-RESOLUTION TRANSMISSION ELECTRON MICROSCOPE

We have recently acquired state-of-the-art aberration-corrected high-resolution transmission electron microscope (TITAN3 TM 80-300) from FEI Company, Netherlands. This particular microscope has both Cs corrector (spherical aberration, for HRTEM) and probe corrector (for HAADF-STEM) in order to achieve spatial resolution ~ 0.8 Å during imaging of crystals. In EELS mode, energy resolution better than 0.2 eV allows the study of fine details of electronic structure near and extended regions of the absorption edge, providing a wide range of information such as coordination, charge state, bonding environment, and electronic charge density for an atom. Capability of simultaneous imaging in the sub-angstrom level and spectroscopy (atom by atom) is an extremely powerful tool to get direct insight into many of the concepts and controversial issues associated with solid state physics through structure (both crystallographic and electronic) and property correlation.

EELS FROM MAGNETIC THIN FILM AND NANOSTRUCTURES

EELS can also be utilized to obtain both magnetic linear and circular dichroic signals from ferromagnetic and paramagnetic materials in order to experimentally evaluate the origin of magnetization in complex magnetic materials. Aberration-corrected microscopy allows us to select very small specific area of a given sample to deduce such properties. This new technique might unravel the complexity in phase separation in highly correlated electron systems, complete understanding of certain magnetic phenomena in manganites, dilute magnetic semiconductors, metamagnetic materials and ferromagnetic/antiferromagnetic interfaces in magnetic multilayers which are important for the rapidly growing field of spintronics. Electron magnetic circular dichroism (EMCD) in a TEM is a new idea and more work needs to be done both in experimentation and simulation before it can be turned into practice.

SEMICONDUCTOR NANOSTRUCTURES

Semiconductor nanostructures – mainly nano-wires, nano-rods and quantum dots – offer many novel properties which can be exploited for many different applications. InGaN, AlGaN, ZnO, and BCN-based semiconductor nanostructures may have improved performance in green light emission, high performance solar cells, hydrogen generation devices, UV emitters, and solar blind photo detectors. Many of the obstacles associated with hetero epitaxial growth can be overcome being able to fabricate them in well aligned nano-wires (and nano-rod or pillar, two dimensional quantum confinement) as well as quantum dots (three dimensional quantum confinement) configurations.

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SOFT MATERIALS

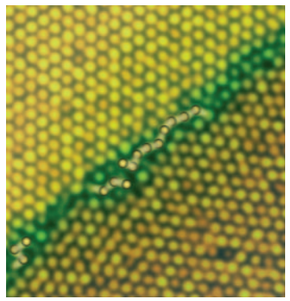
Our Group's research interests are in experimental soft condensed matter physics. A few examples of soft condensed matter (SCM) systems that we encounter daily include moisturizing lotions, emulsions, pastes and bacteria. SCM systems are at the forefront of existing and emerging technology, like flexible displays using e-inks. The microstructure of SCM, ranging in size from tens of nanometers to a few microns, completely determines the macroscopic behavior. Understanding the microstructure-bulk behavior link is essential from a scientific and technological standpoint and is necessary for designing novel SCM materials with tailor-made properties.

The research problems we address falls broadly into two categories. One, the statics and dynamics of self-assembly in colloids and surfactant systems. Two, the response of soft materials to external perturbations such as shear, gravitation, electric and magnetic fields. The techniques that we use to study our systems include rheology, light scattering, confocal microscopy, and optical tweezers.

GRAIN BOUNDARIES

From aluminum coat hangers to aerospace alloys, most materials that we encounter are polycrystalline. Grain boundaries (GBs) – thin interfaces that separate adjacent regions with different crystallographic orientation in polycrystals – play a pivotal role in determining the macroscopic properties of these materials. Computer simulations have been extensively used to study the dynamics of GBs, but these are often limited to temperatures and driving forces much higher than those typically encountered in atomic experiments. Further, the short spatial and temporal scales in atomic systems preclude direct experimental access to GB dynamics. We are currently using high-speed confocal microscopy to directly investigate the dynamics of GBs in a 3-dimensional colloidal polycrystal with single-particle resolution. In a recent study we have shown that GBs share many of the hallmark features of glasses.

Fig. : Confocal microscope image of a colloidal polycrystal. The green region is the grain boundary. Particles at grain boundaries exhibit cooperative dynamics and move in a string-like manner



3D IMAGING OF SOFT MATERIALS UNDER SHEAR

The response of soft materials to an external perturbation, such as shear, is always accompanied by a microstructural change. In our Group, we have recently set up a confocal-rheometer facility that allows us to get simultaneous 3D structural information of soft materials when they are subjected to a shear force. A research problem we are currently working on is to understand the yielding behavior of soft colloidal crystals.

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PHYSICS OF SOFT MATTER

What is common between a bar of soap or chocolate, a bowl of ice-cream or mayonnaise, the flow of toothpaste, fresh concrete or a puddle of mud – objects that we encounter in everyday life? The physical and mechanical properties of these 'soft' materials are governed by structures on the mesoscopic scale (1nm – 1 μm). My research interest lies in understanding the structure, phase behavior, and non-equilibrium phenomena of some of these soft matter systems comprising ordered mesophases of amphiphilic systems, particle/ protein stabilized emulsions, colloidal gels, active gels formed by biopolymer networks, and Langmuir monolayers at fluid interfaces.

We have shown that the interplay between shear flow and structure under an externally imposed shear field in such systems can give rise to many interesting features in non-equilibrium physics such as shear thickening in fractal flocs of nanotube suspensions, shear-banding in Langmuir monolayers, shear-induced phase transitions in lyotropic surfactant systems, and jamming at particle/ surfactant stabilized fluid interfaces.

Different tools such as static or dynamic light scattering, optical imaging or small angle x-ray diffraction (SAXS) methods combined with rheology (Rheo-SAXS) are used to study the correlation between structure, dynamics and mechanical response of these soft materials in the bulk and at fluid interfaces. In addition, SAXS and Rheo-SAXS experiments in synchrotron beamlines at Soleil, France, and the Petra-III DESY, Hamburg, Germany, are being used to study the phase behaviour and non-equilibrium phase transitions in liquid crystalline phases of lyotropic systems.

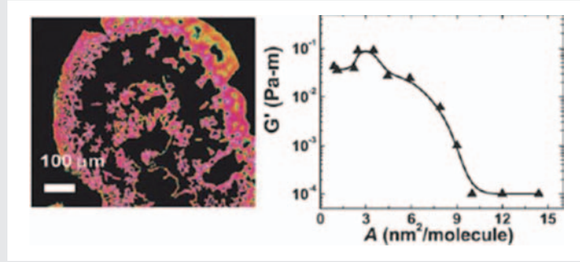

Fig. 1: Interfacial elastic modulus of alamecithin monolayer at au-water interface increases with surface concentration

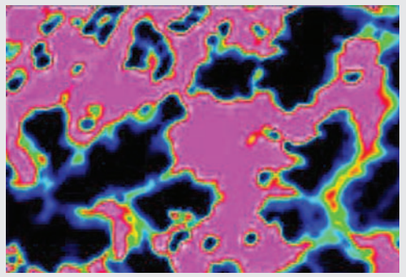

Fig. 2: Shear-thickened state of CNT suspension

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Sridhar Rajaram

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ORGANIC MATERIALS AND ORGANOCATALYSIS

The high cost associated with the production of inorganic semiconductors has been a barrier for the development of low-cost electronic devices. Solution-processable organic semiconductors provide a cost-effective alternative. However, in order to fully realise the promise of low-cost electronics, the performance of organic electronic devices has to be improved. Our Group will be addressing this area through the toolkit of synthetic chemistry.

The approaches we will utilise are as follows:

1. The synthesis of patternable polymers for applications in Organic Light Emitting Diode (OLED), Field Effect Transistors (FET), and in Solar Cells.
2. The development of novel polymeric materials that can self-assemble into nanoscale domains.
3. The synthesis of novel organic-inorganic hybrid materials.

ORGANOCATALYSIS

Conventional asymmetric catalysis has relied on the use of chiral organometallic catalysts. Inspired by enzymes, a number of groups have recently developed small molecules that effect enantioselective transformation in the absence of metals. Our Group will focus on the development of simple catalytic systems to explore novel reactivity patterns. Mechanistic studies will be conducted to evaluate the role of catalysts and guide the development of new catalysts.

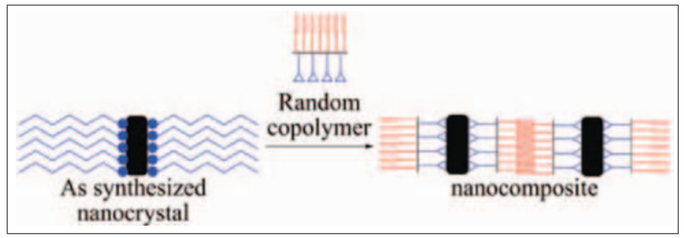
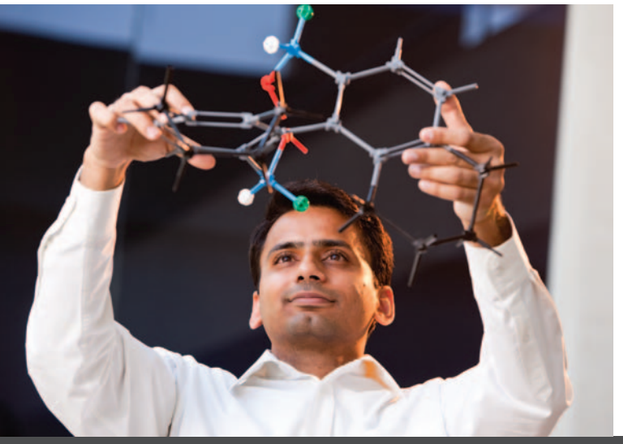


Fig. 1: Effect of the position of Chlorine (green ball) in the small molecule (a potential drug) on the binding with p300 (a hystone acetyl transferase, HAT)protein demonstrated by SERS



KEY PUBLICATIONS

S Rajaram, PA Armstrong, BJ Kim, and JMJ Fréchet, *Effect of a Diblock Copolymer on Blend Morphology and Performance of Poly(3-hexylthiophene): Perylene Diimide Solar Cells,* **Chem. Mater. 21,** 1775-1777 (2009).

S Rajaram, TL Choi, M Rolandi, and JMJ Fréchet, *Synthesis of Dendronized Diblock Copolymers via Ring Opening Metathesis Polymerization and their Visualization Using Atomic Force Microscopy,* **J. Am. Chem. Soc. 129,** 9619-9621 (2007).

S Rajaram, and MS Sigman, *Design of Hydrogen Bond Catalysts Based on a Modular Oxazoline Template: Application to an Enantioselective Hetero Diels-Alder Reaction,* **Org. Lett. 7,** 5473-5475, (2005).

S Rajaram, and MS Sigman, *Modular Synthesis of Amine Functionalized Oxazolines,* **Org. Lett. 4,** 3399 (2002).

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PHYSICS AND CHEMISTRY OF NANOMATERIALS

The research in her Group is focused on the syntheses and study of electronic and optical properties of semiconductor nanocrystals and nanoscale assemblies. The interest in these quantum confined systems stem from the fact that these tiny fragments exhibit a wide range of properties that can be tuned by changing the size of the particles. In certain cases, these tiny fragments are also known to show properties that are not observed in bulk materials.

The ability to precisely control the composition, size, and shape of the nanocrystals provides great flexibility in engineering their electronic and optical properties. Tunable dimensions and shapes of the individual particles as well as the ease of manipulating them into a complex interacting structure make colloidal nanocrystals well-suited for studies of size- and structure-dependent quantum-mechanical interactions. Understanding the mechanisms at work in these tiny particles has important implications in the areas of photovoltaics, displays, memory storage, and optoelectronic devices.

Fundamental research into the synthesis of these nanocrystals by various wet chemical routes, as well as studying and understanding the size-dependent electronic, optical, and magnetic properties of these materials constitutes the major research activity in this Group.

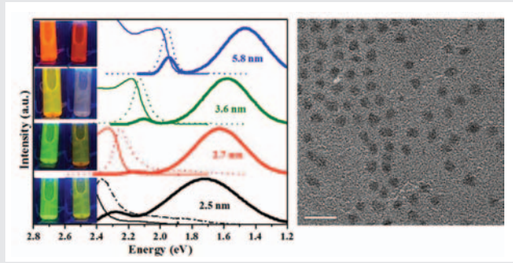

Fig. : Typical absorption, fluorescence and TEM images of copper doped and undoped nanocrystals of different sizes

KEY PUBLICATIONS

R Viswanatha, S Brovelli, A Pandey, SA Crooker, and V. I. Klimov, *Copper-Doped Inverted Core Shell Nanocrystals with Permanent Optically Active Holes,* **NanoLetters 11,** 4753 (2011).

R Viswanatha, JM Pietryga, VI Klimov, and SA Crooker, *Spin-polarized Mn2+ emission from Mn-doped colloidal nanocrystals,* **Physical Review Letters 107,** 67402 (2011).

S Brovelli, RD Schaller, SA Crooker, F Garcia-Santamaria, Y Chen, R Viswanatha, JA Hollingsworth, H Htoon, and VI Klimov, *New Paradigm for Controlling Exciton Dynamics Via Engineered Electron-Hole Exchange Interaction,* **Nature Communications 2,** 280 (2011).

PK Santra, R Viswanatha, SM Daniels, NL Pickett, JM Smith, and DD Sarma, *Investigation of the Internal Heterostructure of Highly Luminescent Quantum Dot-Quantum Well Nanocrystals,* **Journal of American Chemical Society 131,** 470 (2009).

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MOLECULAR BIOLOGY AND GENETICS UNIT

RECENT Ph.D. & M.S. THESES (2011-2012)

- Genetic and epigenetic factors determining centromere structure and function in Candida species (Jitendra Thakur, Ph.D., 2011)
- Insights into the role of Brdt in chromatin remodeling during rat spermiogenesis (Surbhi Dhar, Ph.D., 2011)
- Safety, efficacy and immunological evaluation of a polyherbal formulation against HIV-AIDS in an Open-label Clinical Trial (Mangaiarkarasi A, Ph.D., 2011)
- Structure-function studies on three members of the Haloacid Dehalogenase (HAD) superfamily of enzymes (Bharath S, Ph.D., 2011)
- Rudhira is a cytoskeletal protein that regulates directional cell migration during vascular development (Mamta Jain, Ph.D., 2012)
- Biochemical characterization of Plasmodium falciparum Glutamine Amidotransferase and Adenosine Triphosphate Pyrophosphatase: domains of GMP Synthetase (T. Lakshmi Prasoona, M.S., 2012)
- Functional analysis of Centromeres and Centromere Associated Histone H3 in two Budding yeasts, Candida albicans and Saccharomyces castellii (V. Sivani, M.S., 2012)

Molecular Biology and Genetics Unit (MBGU) is well-recognized for its research programmes and training in broad areas of biological and biomedical sciences. Research in its nine laboratories spans diverse areas of modern biology with emphasis on biomedicine. The current areas of research include infectious diseases, cancer genomics, human neurological disorders, mammalian stem cells, cardiovascular development, transcription regulation and mechanism of chromosome segregation.

Research in the MBGU labs has been supported by grants from several funding agencies as well as from the biotechnology industry. In the last five years or so, there has been an active exchange of scientific ideas among this MBGU faculty and colleagues who are chemists, physicists and engineers at the centre. Each laboratory in the unit is well equipped with their individual requirements; certain major research facilities which include a multi-photon confocal microscope, mass-spectrometer, microarray scanners, DNA sequencing machine, are run as shared facilities. A central animal facility provides suitably regulated access to small animals, rats, mice and rabbits and, a central computer laboratory in the centre gives high-speed internet access and technical support to the unit.

MBGU attracts some of the best students from all over the country. Students for the Ph.D., Integrated-Ph.D., MS-Ph.D., POBE and SRF programmes in MBGU are selected through competitive national-level selection process. Our academic programmes aim to provide training in a broad range of genetic, biochemical, cell and developmental biology approaches for basic and translational research. The essence of these programmes is to provide students, ample flexibility and opportunity for pursuing a contemporary research theme, and a broad-based training in multidisciplinary research areas. MBGU has a vibrant and interactive research atmosphere for its students, who find themselves immersed in multiple academic activities including research work presentations, journal club discussions, training workshops, thematic conferences and lectures by visiting scientists, throughout the year. Students are encouraged and supported to present their results at the scientific meetings. Students who graduate from the department have gone on to join in the academia as well as industry.

MBGU faculty can be directly contacted through our web site www.jncasr.ac.in/mbgu

Anuranjan Anand

ANURANJAN ANAND OBTAINED HIS Ph.D. FROM INDIAN INSTITUTE OF SCIENCE, BANGALORE AND POST-DOCTORAL TRAINING AT STANFORD UNIVERSITY, PALO ALTO, USA. HE JOINED THIS CENTRE IN 1997.

MOLECULAR AND CELLULAR MECHANISMS OF HUMAN GENETIC DISORDERS

The main focus of research in my laboratory is to explore the molecular and cellular basis of common human disorders: genetic generalized epilepsies, sensory epilepsies, neuropsychiatric disorders and congenital hearing loss. We have discovered several novel genes or genetic loci for epilepsy (2q33-q36, 3q13-q21, 5q12-q14, 5q33-q35, 4q24-q28, 10q21-q22), deafness (9p31-21, 11p14-q12, 18q 12-21), bipolar affective disorder (1p32.1, 6p24.3-ter). These genes/loci are currently being studied to isolate disease-causing mutations. We have also identified a wide spectrum of pathogenic mutations in several deafness-causing genes and examined the molecular basis of sensorineural, non-syndromic hearing impairment in Indian populations. The identification of over four dozen pathogenic mutations in the *Cx26, Cx30, TMPRSS3, TMC1, HAR, CDH23, SLC26A4, OTOF* and *TMIE* genes has substantially extended our understanding of allelic heterogeneity at these genes and provided a number of new alleles for potential use in cell biological, biochemical and structure-function correlation studies. Knowledge of the relative contributions of these genes to the load of hereditary hearing loss has helped devise a 'genetic algorithm' that has important utility for early detection of the disorder and implementation of suitable intervention therapies.

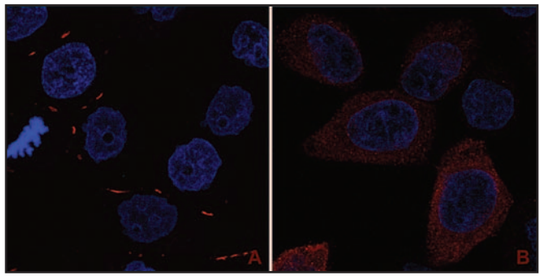

Fig. : Sub-cellular localization of the wild type and mutant CONNEXIN 26 proteins. Wild type CONNEXIN exhibits characteristic gap-junction plaques at the junction of two contacting cells (A). Localization of the defective CONNEXIN occurs in the cytoplasm and no gap-junction plaques are observed (B)

KEY PUBLICATIONS

R Ratnapriya, J Vijai, J Kadandale, Rajesh Iyer, R Radhakrishnan and A Anand, *A new locus for juvenile myoclonic epilepsy maps at 2q33-q36.* **Human Genetics (2010)**

R Ratnapriya, P Satishchandra, D Kumar, G Gadre, R Reddy and A Anand, *A locus for autosomal dominant reflex epilepsy precipitated by hot water maps at chromosome 10q21.3-q22.3.* **Human Genetics (2009)**

R Ratnapriya, P Satishchandra, D Kumar, G Gadre and A Anand, *Familial autosomal dominant reflex epilepsy triggered by hot water maps to 4q24-q28.* **Human Genetics (2009)**

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MOLECULAR PARASITOLOGY AND MOLECULAR ENZYMOLOGY

My laboratory focuses primarily on molecular enzymology and specific aspects of metabolism in *Plasmodium falciparum.* The malaria-causing *Plasmodium falciparum* is one of the most pathogenic microbes that continues to pose health hazards in many parts of the world. As a parasite that is largely intracellular, residing within host cells, it has evolved a unique set of biochemical pathways to adapt to the milieu of its growth. Metabolic pathways that are indispensable for parasite survival serve as ideal targets for the development of new antimalarials. The purine salvage pathway is one such potential target as it provides the sole source of purine nucleotides to the parasite.

Our studies are focused on the characterization of purine salvage enzymes, hypoxanthine guanine phosphoribosyltransferase, adenylosuccinate synthetase, adenylosuccinate lyase, GMP synthetase and 5' purine nucleotidases of *P. falciparum.* Comparative studies on human homologs have permitted the identification of structural and functional characteristics specific to the enzymes from the two organisms. We also study the homologs of these enzymes from the thermophilic archea *Methanocaldococcus jannaschii* to understand the effect of temperature on catalysis and structural stability. Tools of molecular biology, enzymology (steady state and burst phase kinetics, and simulation of kinetic mechanisms using appropriate models), protein chemistry (chemical modification, and mass spectrometric analysis) and biophysics (fluorescence and circular dichroism spectroscopy, and x-ray crystallography) are used to address different issues of protein structure and function.

The laboratory has also been examining the crosstalk between purine nucleotide and tricarboxylic acid (TCA) cycles as the adenylate arm of purine nucleotide synthesis generates fumarate. *P. falciparum,* during its intraerythrocytic stages is microaerophilic in nature with the mitochondria not contributing significantly to ATP production. However, the parasite expresses the enzymes of the TCA cycle and those of the electron transport chain indicating an alternate function for these pathways. In this context, the fate of metabolites produced by diverse pathways that feed into the TCA cycle merits study. Examination of novel metabolic features in pathogenic organisms should aid in the development of therapeutic agents.

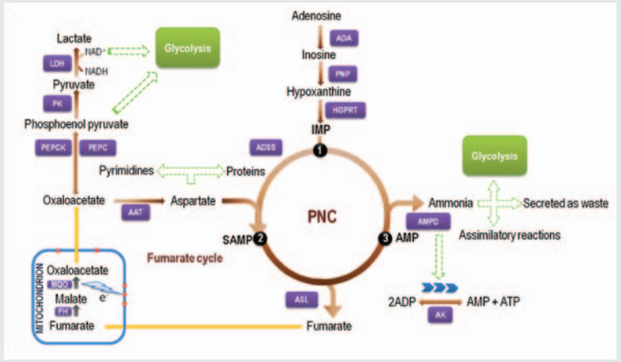

Fig. : Cross talk between purine nucleotide metabolism and mitochondrial pathways in *Plasmodium falciparum*

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MOLECULAR, GENETIC AND DEVELOPMENTAL ANALYSIS OF THE CARDIOVASCULAR SYSTEM

Cardiovascular defects and disease are the leading cause of prenatal, postnatal and adult mortality. The promise of stem cells and regenerative medicine is to repair and restore defective or diseased parts of the human body. Our aim is to improve understanding of cardiovascular development and physiology as it has application in prevention of congenital defects as well as for regenerative therapies that promote stem cell-mediated repair.

While several signaling pathways and their transcriptional effectors are known, there is limited information about the complex cytoplasmic machinery that regulates and effects cellular processes. Using an unbiased gene expression-based approach we identified novel genes that control cellular traffic (gene: asrij) and cytoskeletal changes (gene: rudhira) in the cardiovasculature. We use multiple model systems and cell lineages with a variety of approaches to study these molecules and gain insight into cardiovascular lineage specification, differentiation and disease development. We have derived human embryonic stem (hES) cell lines as model for human development and induced pluripotent stem (iPS) cells as disease models. We also improved protocols to generate cardiomyocytes from these hES cells.

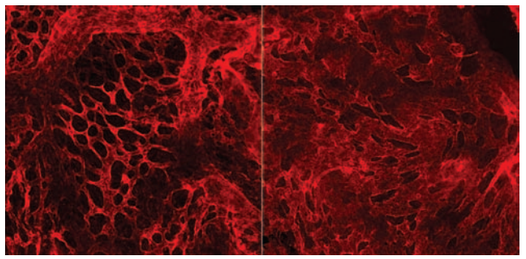

Fig. : Intricate network of blood vessels (red) seen in a normal mouse embryo (left) is unpatterned and disorganized in a *rudhira* null mutant embryo (right)

KEY PUBLICATIONS

Sudhir H Ranganath, Oren Levy, Maneesha S Inamdar and Jeffrey Karp, *Harnessing the Mesenchymal Stem Cell Secretome for the Treatment of Cardiovascular Disease,* **Cell Stem Cell 10,** 244-258 (2012).

Mamta Jain, Ganesh P Bhat, VijayRaghavan K, and Inamdar M S, *Rudhira/BCAS3 is a cytoskeletal protein that controls Cdc42 activation and directional cell migration during angiogenesis,* **Experimental Cell Research 318 (6),** (2012).

The International Stem Cell Initiative, *Screening a large, ethnically diverse population of human embryonic stem cells identifies a chromosome 20 minimal amplicon that confers a growth advantage,* **Nature Biotechnology 29,** 1132–1144, (2011).

Kulkarni V, Khadilkar, R, Srivathsa, M S and Inamdar M S, *Asrij Maintains the Stem Cell Niche and controls differentiation during Drosophila Lymph Gland Hematopoiesis,* **PLoS ONE 6(11)**): e27667, (2011).

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TRANSCRIPTION REGULATION AND CHROMATIN DYNAMICS: IMPLICATIONS IN DISEASE AND POTENTIAL THERAPEUTICS

CHROMATIN DYNAMICS AND TRANSCRIPTION REGULATION

a) Non-histone nuclear proteins and chromatin dynamics

Highly abundant nuclear proteins dynamically interact with chromatin and confer functional fluidity. These include different histone interacting proteins such as PC4, HMGs, HP1 etc. We investigate the role of human PC4 and its interacting partners in the chromatin organization and thereby transcription regulation in the context of diseases such as cancer and AIDS. Furthermore, involvement of microRNA in the regulation of these proteins and chromatin modifying enzymes are also being investigated.

b) Role of histone chaperone in transcriptional regulation

Histone chaperones are a group of proteins which play important role in histone metabolism such as assembly and disassembly of nucleosomes during different physiological processes. Thus these proteins are important regulators of transcription. We are focusing on the mechanism of transcriptional activation by the human histone chaperone NPM1 and its relevance in disease manifestation.

EPIGENETIC LANGUAGE OF TRANSCRIPTIONAL ACTIVATION

We are trying to understand the language of epigenetic marks that underlie the signal towards transcriptional activation under normal conditions. We are also trying to correlate these epigenetic phenomena with pathophysiological states such as cancer and AIDS.

CHEMICAL BIOLOGY APPROACH TO UNDERSTAND EPIGENETIC PHENOMENA

Work in our laboratory has immensely contributed to the area of modulators of chromatin modifying enzymes. These modulators have helped in understanding the epigenetic phenomena underlying several physiological and pathophysiological processes. The present focus of the laboratory is to find out the non-ATP analog inhibitors of Aurora Kinases, more potent small molecule modulators of Histone Acetyltransferases and Arginine Methyltransferases from natural sources.

NANOBIOTECHNOLOGY APPROACH FOR TARGETED THERAPY

In collaboration with the CPMU, JNCASR we are actively working in the area of nanobiotechnology. The major emphases have been given to the possible utilization of our recently discovered carbon nanospheres. The mechanism of its ability to cross the blood-brain barrier, delivery of the HAT activator molecule in the mammalian brain and targeted delivery of anti-neoplastic therapeutics in the solid tumor targeting the epigenetic modifications are the major focus of our laboratory.

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AUTOPHAGY AND AUTOPHAGY RELATED PATHWAYS

Every cell in our body is equipped with a form of house-cleaning machinery called autophagy. Autophagy is universally present in all eukaryotic cells, from yeast to humans. During nutrient starvation, autophagic processes promote cell survival by degrading superfluous cytoplasmic proteins and organelles.

A key morphological event during autophagy (macroautophagy) is the formation of a double membrane structure called the phagophore, that engulfs the cargo destined for lysosomal or vacuolar degradation. Cargoes include bulk cytosol, protein aggregates, organelles such as peroxisomes and mitochondria, and intracellular pathogens such as bacteria and viruses. Of these cargoes, several intracellular pathogens including bacteria (like *Salmonella, Shigella, Mycobacterium,* and Group A *Streptococcus*) and viruses (like herpes simplex virus and HIV) subvert autophagy to prevent their elimination by degradation in host lysosomal compartments. Autophagy also plays a neuroprotective role, as it clears large aggregates of mutant polyubiquitylated proteins resistant to proteasomal degradation. Furthermore, apart from neurodegenerative and infectious diseases, autophagy has been shown to be involved in heart diseases, atherosclerosis, certain myopathies, innate and adaptive immune responses, Crohn's disease, and cancer. Recently, autophagy has been shown to play an unexpected role in unconventional secretion of proteins. However, much of the molecular details of how this is accomplished is yet to be unraveled.

Thus, targeting autophagy is a potentially exciting avenue that is just beginning to be exploited for disease and cancer cures. Recent studies have shown that modulating autophagy has positive outcomes in the diseases mentioned above. For example, regulating autophagic activity, either genetically or biochemically, has resulted in increased killing of intracellular mycobacteria. Pharmacologically, small molecules targeting autophagy have been shown to be effective in clearing protein aggregates in a Huntington disease model system. However, lack of effective and robust screening methods have limited the discovery of candidate molecules. Novel sensitive assays that monitor autophagy rates are needed to discover new candidate molecules. Thus, pharmacological intervention of autophagy is extremely desirable considering the myriad of physiological and pathological processes it is involved in.

The laboratory currently focuses on using several yeast as a model system to explore autophagy and autophagy-related pathways. Using conventional and novel assays, we are investigating specific steps in autophagy, such as signaling, transport and fusion. The information gained from such work will be used to study the role of autophagy in the host-pathogen interactions.

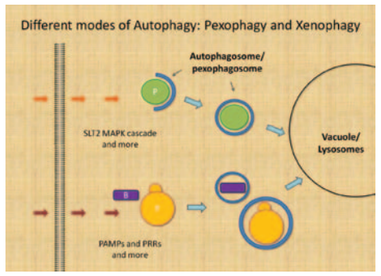

Fig. : Schematic comparison between macroautophagic degradation of peroxisomes (P) (pexophagy) and macroautophagic elimination of pathogens (B, Y) (xenophagy)

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M R S Rao

MRS RAO OBTAINED HIS Ph.D. AT THE INDIAN INSTITUTE OF SCIENCE. HE WAS A RESEARCH ASSOCIATE AND ASSISTANT PROFESSOR AT BAYLOR COLLEGE OF MEDICINE, BEFORE RETURNING TO IISC. HE WAS PROFESSOR AND CHAIRMAN OF THE DEPARTMENT OF BIOCHEMISTRY, IISC. HE IS NOW THE PRESIDENT OF JNCASR.

CHROMATIN BIOLOGY AND GENOMICS

We have developed a method for culturing haploid round spermatids in vitro for molecular manipulation. Remodeling assays using these cultured cells have shown an acetylation dependent but ATP independent chromatin reorganization property of Brdt in haploid round spermatids. Brdt interacts with Samrce 1, a member of the SWI/SNF family. The genomic organization of smarce 1 identified two splice variants expressed during spermatogenesis. Nucleosomal histones are replaced by transition proteins, TP1, TP2 and TP4 in the later stages of spermiogenesis. We have observed that in addition to acetylation, TP2 also undergoes methylation by PRMT4 (CARM1). The amino acid residues that undergo methylation have now been mapped both by mutation analysis as well as by Mass spectrometry. The functional significance of this post translation modification of TP2 is now being investigated.

Non coding RNAs play a pivotal role in processes like transcriptional and post transcriptional regulation, mRNA and protein stability. One such non-coding RNA, mrhl, is encoded in the mouse genome that is nuclear restricted. Expression of genes belonging to cell adhesion, cell signaling and development and differentiation are significantly perturbed in the mrhl RNA down regulated cells, among which many were of the wnt signaling pathway. Many of the transcription factors were also differentially regulated under these conditions one among which is Tcf4 which activates downstream target genes of wnt signaling pathway. Mrhl RNA interacts with p68, one of the RNA binding proteins in the nucleus, which mediates the wnt signaling activation. We have proposed that mrhl RNA is a negative regulator of wnt signaling in spermatogenic cells.

AEBP1 is a transcriptional repressor that is involved in adipogenesis, which binds to aAE-1 element present in the proximal promoter of aP2 gene that code for fatty acid binding protein (FABP4). To elucidate the role of AEBP1 over expression in glioblastoma, we employed complementary gene silencing approach to identify the genes that are perturbed in a glioma cell line (U87MG). Genes which were differentially regulated under these conditions belonged to different GO categories such as transcription regulation, cell growth, proliferation and differentiation, apoptosis and signaling etc. Upon AEBP1 silencing, both cellular proliferation and survival were affected in U87MG and U138MG cell lines, a significant percentage of which was directed towards apoptosis.

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THE HIV-1 SUBTYPE-C STRAIN: SUCCESS STORY OF THE FITTEST VIRAL SUBTYPE

Among the various HIV-1 genetic subtypes, subtype-C is the most predominant viral family causing half the global infections. What makes subtype-C the super HIV? Do the diverse viral subtypes differ in their pathogenic properties? We believe so. For instance, we proposed that the viral strains of subtype-C are incapable of causing neuron death in the human brain primarily as a consequence of a single amino acid variation in the viral factor Tat.

Where is the HIV evolution headed – towards less pathogenic viral strains? We think so. We have found that, over the past decade, highly infectious HIV strains have originated in India and South Africa and have been replacing the circulating viral strains at a rapid pace. The novel strains, however, may not be more pathogenic.

We all desperately need superior viral control measures. Could the alternative medicines of India be a source of hope? Looks like the case. In a pilot human clinical trial using a poly-herbal formulation in 32 subjects, we found stabilized clinical profile in a two-year study.

Work in the laboratory also focuses on breaking the HIV viral latency, DNA vaccine development and studying the dominant host immune responses to HIV.

KEY PUBLICATIONS

Venkatesh Prasanna Kashi, Rajesh Abraham Jacob, Siddhartha Paul, Kaustuv Nayak, Bhuthiah Satish, Soumya Swaminathan, Kadappa S Satish, Udaykumar Ranga, *HIV-1 Tat-specific IgG antibodies in high-responders target a B-cell epitope in the cysteine-rich domain and block extracellular Tat efficiently,* **Vaccine 27,** 6739-6747 (2009).

Prasanta K Dash, Nagadenahalli B Siddappa, Asokan Mangaiarkarasi, Aruna V Mahendarkar, Padmanabhan Roshan, Krishnamurthy Kumar Anand, Anita Mahadevan, Parthasarathy Satishchandra, Susarla K Shankar, Vinayaka R Prasad, and Udaykumar Ranga, *Exceptional molecular and coreceptor requirement properties of molecular clones isolated from an Human Immunodeficiency Virus Type-1 subtype C infection,* **Retrovirology 5,** 25 (2008).

Nagadenahalli Byrareddy Siddappa, Mohanram Venkatramanan, Prasanna Venkatesh, Mohanbabu Vijayamma Janki, Narayana Jayasuryan, Anita Desai, Vasanthapuram Ravi, and Udaykumar Ranga, *Transactivation and signaling functions of Tat are not correlated: biological and immunological characterization of HIV-1 subtype-C Tat protein,* **Retrovirology 3,** 53 (2006).

Nagadenahalli Byrareddy Siddappa, B Prashant, Kumar Dash, Anita Mahadevan, Anita Desai, Narayana Jayasuryan, Vasanthapuram Ravi, Parthasarathy Satishchandrad, Susarla K Shankar, and Udaykumar Ranga, *Identification of unique B/ C recombinant strains of HIV-1 in the southern state of Karnataka,* **India, AIDS 19,** 1426-1429 (2005).

Udaykumar Ranga, Raj Shankarappa, Nagadenahalli B Siddappa, Lakshmi Ramakrishna, Ramalingam Nagendran, Marthandan Mahalingam, Anita Mahadevan, Narayana Jayasuryan, Parthasarathy Satishchandra, Susarla K Shankar, and Vinayaka R Prasad, *Tat Protein of Human Immunodeficiency Virus Type 1 Subtype C Strains Is a Defective Chemokine,* **Journal of Virology 78,** 2586-2590 (2004).

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Kaustuv Sanyal

KAUSTUV SANYAL OBTAINED HIS Ph.D. IN YEAST GENETICS FROM THE BOSE INSTITUTE, KOLKATA. HE UNDERWENT POST-DOCTORAL TRAINING ON CENTROMERE STRUCTURE-FUNCTION ANALYSIS AT THE UNIVERSITY OF CALIFORNIA, SANTA BARBARA, BEFORE JOINING JNCASR.

GENETIC AND EPIGENETIC DEFINITION OF CENTROMERES

Several proteins bind to centromere (CEN) DNA to form kinetochores, which help in the attachment of chromosomes to the spindle microtubules during mitosis and meiosis. The main focus of our laboratory is to understand the mechanism of chromosome segregation in pathogenic yeasts. Several lines of evidence suggest that CEN formation in most organisms is not entirely a sequence-dependent phenomenon. By mapping sites of neocentromere formation, we discovered that a three-dimensional chromosomal scaffold is probably an epigenetic factor that determines CEN identity. Based on a series of experimental evidence, we also propose that presence of an early replicating origin also determines centromere location. Functional cloning and comparative genomics studies in our laboratory revealed the CEN sequence and DNA elements are rapidly evolving although the relative location of the CEN region remains evolutionarily conserved in related species. Finally, we showed that an interdependent protein circuitry ensures assembly and stability of the functional kinetochore on CEN DNA.

Our key areas of interest are:
- Mechanism of centromeric chromatin formation
- Evolution of centromere structural elements
- Relation between RNAi machinery and transcriptional silencing
- Epigenetic coding of the functional genome by histone H3 variants

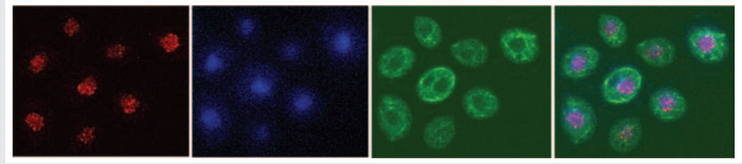

Fig. : Centromeres in Cryptococcus neformans, a human pathogen, that causes fungal meningitis

KEY PUBLICATIONS

K Sanyal, *How do microbial pathogens make CENs?* Invited review, **PLoS Pathogens** (February 2012).

B Roy, and K Sanyal, *Diversity in requirement of genetic and epigenetic factors for centromere function in fungi,* Invited review, **Eukaryot Cell 10,** 1384-1395.

J Thakur, and K Sanyal, *The Essentiality of the Fungus-Specific Dam1 Complex Is Correlated with a One-Kinetochore-One-Microtubule Interaction Present throughout the Cell Cycle,* Independent of the Nature of a Centromere, Cover article, **Eukaryot Cell 10,** 1295-1305.

B Roy, LS Burrack, MA Lone, J Berman, and K Sanyal, *CaMtw1, a member of the evolutionarily conserved Mis12 kinetochore protein family, is required for efficient inner kinetochore assembly in the pathogenic yeast, Candida albicans,* **Mol. Microbiol. 80,** 14-32.

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MECHANISMS UNDERLYING HOST-PATHOGEN INTERACTIONS IN MALARIA

Plasmodium falciparum, which causes the most fatal form of human malaria kills 1-3 million people each year. The absence of a malaria vaccine, and its widespread resistance to drugs leads us to rely on an increased understanding of *Plasmodium falciparum* biology. *Plasmodium* possesses unique qualities responsible for the virulence of the disease and immune invasion. Deciphering hostpathogen interactions offers the hope of a malaria cure. To this end, our laboratory uses proteomics, genomics, molecular biology, cell biology and Systems-Biology approaches for detailed delineation of parasite biology and host-pathogen interactions.

Plasmodium-DERIVED PROTEINS RESPONSIBLE FOR MALARIA VIRULENCE AND ACTIVE SIGNALING

After the invasion of erythrocytes, the human malaria parasite resides within a parasitophorous vacuole and develops from ring to schizont stage. The virulence of this organism is due in part to the way in which it modifies the membrane of the infected erythrocytes it grows in.

These virulence factors include PfEMP1, ETRAMPS, and kinases of the FIKK family. PfEMP1 molecules are trafficked to the erythrocyte plasma membrane, where they mediate adhesion to host receptors on the vascular endothelium and other cells, while members of FIKK proteins and ETRAMPS are involved in the remodelling of the erythrocyte surface and active signaling between host and parasite.

HOST FACTORS INVOLVED IN RESISTANCE OR SUSCEPTIBILITY TO MALARIA

Plasmodium falciparum has a profound effect on the evolution of the human genome. Populations historically exposed to *Plasmodium falciparum* malaria demonstrate resistance to severe clinical forms of malaria. We are attempting to confirm the host-associated factors in a large-scale, case-control study of severe malaria in South India.

THE SYSTEMS-BIOLOGY APPROACH TO UNDERSTAND MOLECULAR CORRELATES FOR PATHOGENESIS OF CEREBRAL VS UNCOMPLICATED MALARIA

The patients infected with *P.falciparum* present with a range of outcomes, from asymptomatic parasitemia to severe disease leading to death further points to poorly and partially defined mechanisms of the host and parasite factors that mediate the severity of the disease.

Severe *falciparum* malaria is a complex of different clinical manifestations leading mainly to cerebral, renal and pulmonary dysfunction. In India, severe *falciparum* malaria is mostly associated with renal and pulmonary complications and rarely with cerebral malaria. The genetic and molecular basis of this diversity remains unknown.

We are trying to identify the parasite factors responsible for virulence and host-parasite interactions by characterization in complete in vivo parasite protein-protein interactions network by 'Systems-Biology'.

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NEW CHEMISTRY UNIT

RECENT THESIS (2011-2012)

- Investigations of the $Al_{1-x}GaxFeO_3$ Family and other Oxide Materials (Ajmala Shireen P, M.S., 2012)

The New Chemistry Unit (NCU) is a relatively new unit currently with eight core faculty members and Prof. C. N. R. Rao as the Chairman. Several faculty members from the other units of the centre are also associated with NCU. The unit works on interdisciplinary aspects of chemical science. The most important areas that are actively pursued are at the interface of chemical biology, chemical Science and materials Science. Some of the specific areas of research are Inorganic nanomaterials, carbon based nanomaterials, Chemical storage of hydrogen, organic synthesis, peptides and nucleic acids, biomaterials, organic and supramolecular chemistry, antimicrobial agents, drug discovery, drug delivery systems, patternable polymers, conducting polymers, theoretical chemistry, and catalysis.

The specific research projects involve the synthesis of a host of nanomaterials including organic and inorganic based zero-, one- and two-dimensional materials for applications in magnetic, optical, opto-electronic and electrical devices. Synthesis of extended solids for a range applications, are also being actively pursued. Organic and inorganic synthesis is an integral part of many research groups which involves the asymmetric synthesis, diversity-oriented synthesis, synthesis of heterocyclic compounds, synthesis of organic materials, polymers, nanomaterials etc. Organic-inorganic hybrid materials, inorganic materials for photovoltaic and nonlinear optical applications, nanomaterials for renewable energy, chemical storage of hydrogen in graphene, functional metal-organic frame works for hydrogen storage, catalysis, magnetism and optical properties, polymers and oligomers for solar cells, field effect transistors and organic light emitting diodes, organic functional materials through supramolecular self-assembly, design and synthesis of peptide, protein and nucleic acids based materials for molecular/chiral recognition and biomaterial applications, Chemo(bio)sensors, synthesis of antibacterial agents, developing new drug delivery systems are some of the specific areas. Microscopic understanding of a number such an exotic phenomenon are also being carried out by our theoretical group. The unit has a good analytical facility for complete characterization of various materials perused in our unit. The unit has excellent facilities for computational and theoretical studies to complement the experimental research.

The Unit admits students for the Ph.D degree programme as well as integrated Ph.D in Chemical Sciences. The unit also admits students for integrated MS-Ph.D programme in Chemical Sciences through project oriented chemical education (POCE). The students admitted for these programmes would undergo extensive course work and research training before continuing for dissertation work. NCU maintains strong interactive relationship with other units of the centre.

RESEARCH FACILITIES

NMR Spectrometer
X-Ray Diffractometers
FT-IR, UV-Vis and Fluorescence Spectrometers
Gas Chromatograph Mass Spectrometer (GC-MS)
Liquid Chromatograph Mass Spectrometer (LCMS)
High Performance Liquid Chromatography (HPLC)
Gel Permeation Chromatography (GPC)
Elemental Analyzer (CHNS)
Nano research facilities
Various materials characterization facilities

C N R Rao

CNR RAO, D.Sc. (MYSORE), Ph.D. (PURDUE), Sc.D. (HC), D.Sc. (HC), L.L.D. (HC), D.LITT. (HC), F.R.S., HON. F.R.S.C., HON. F. INST. P. IS A NATIONAL RESEARCH PROFESSOR, LINUS PAULING RESEARCH PROFESSOR AND FOUNDER AND HONORARY PRESIDENT OF JNCASR. HE IS ALSO THE DIRECTOR OF THE INTERNATIONAL CENTRE FOR MATERIALS SCIENCE (ICMS).

EXCITING NEW CHEMISTRY

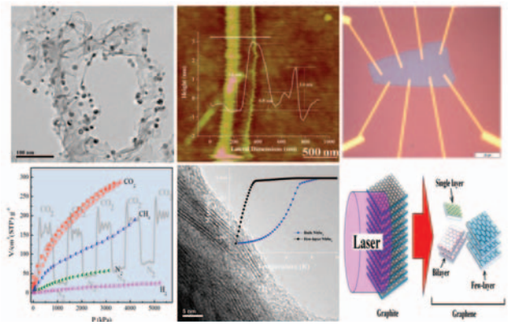
In recent years, the discipline of chemistry has developed many exciting cross-disciplinary aspects. My research interests span solid state and structural chemistry, particularly the phenomena and properties exhibited by transition metal oxide systems, and materials chemistry, especially chemical synthesis and characterisation of designer solids, and nanomaterials with novel structures and properties.

The assembly of nanostructures is critical for device fabrication. Different types of aggregates of nanoparticles have been assembled, which show photoluminescence spectra different from the pristine nanocrystals, and are interpreted in terms of electronic coupling between the nanocrystals. In the area of carbon-based materials, besides finding new methods of preparing different kinds of carbon nanotubes and graphene, separation of metallic and semiconducting single-walled carbon nanotubes (SWNTs) using various chemical techniques have been investigated.

Graphene is a fascinating two-dimensional (2D) carbon material which is the parent of all graphitic carbon forms. There is considerable interest in investigating single-layer, two-layer and few-layer graphenes. Synthesis, characterization, structure, functionalization and properties of graphene are being been carried out. Interestingly, molecular charge-transfer also markedly affects the electronic structure and properties of graphene. Doping graphene with boron (B) and nitrogen (N) as well as the search for graphene analogues have been investigated. In addition, the interaction of graphene with various organic and inorganic systems such as DNA nucleobases and nucleosides have been investigated. Other single-layered 2D structures such as BN and MoS2 have been synthesized using novel chemical procedures. Functionalization and solubilization of inorganic and carbon nanostructures by employing various chemical reagents is an area of extensive research.

Applications of nanomaterials often involve reinforcement in polymer composites, wherein small additions of nanomaterials when incorporated in a polymer matrix lead to large enhancements in mechanical properties. We are evaluating the mechanical properties of these polymer composites by the nanoindentation technique. These show extraordinary synergy, improvement in the stiffness and hardness when compared to those obtained with single nanocarbon reinforcements. Electrical and gas-sensing characteristics of field effect transistors (FETs) based on different nanostructures of oxides, nitrides and other nanomaterials have been another area of interest.

Hybrid organic-inorganic materials of various structures and connectivities are being investigated. Kagome compounds form one such family being studied.



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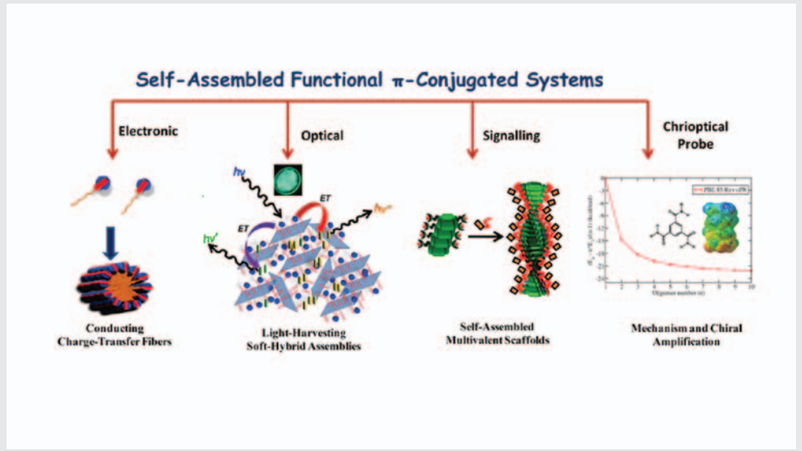
FUNCTIONAL ORGANIC AND SUPRAMOLECULAR MATERIALS

The underlying theme of our research lies at the interface between synthetic efforts on π-conjugated systems and the organization of these molecules using supramolecular self-assembly principles, with the ultimate aim of developing novel functional materials. In our approach we target the electronic, optical and self-assembling properties of the π-conjugated backbone for the design of materials. Our activities towards the electronic functionality focus on the synthesis of novel n-type coronene imide derivatives and on charge-transfer conducting nanofibers via a non-covalent amphiphilic strategy. We target solution processbale fluorescent materials by a non-covalent organic (dyes) –inorganic (organoclay) hybrid co-assembly, which also facilitate



efficient light-harvesting. We further exploit the optical functionally of chromophoric assemblies as multivalent guest scaffolds and for the concept of "supramolecular signal amplification". We also use the chiroptical properties as a probe to study the mechanism of supramolecular self-assembly and chiral amplification such as 'Sergeant and Soldiers' and 'Majority Rules'.
We also have been working non-covalent functionalization of carbon nanomaterials with various aromatic donor and acceptor molecules to form novel class of hybrid materials exhibiting ground- and excited-state charge-transfer, energy transfer and tunable opto-electronic properties. Recently, we have also initiated the design of novel microporous organic polymers.

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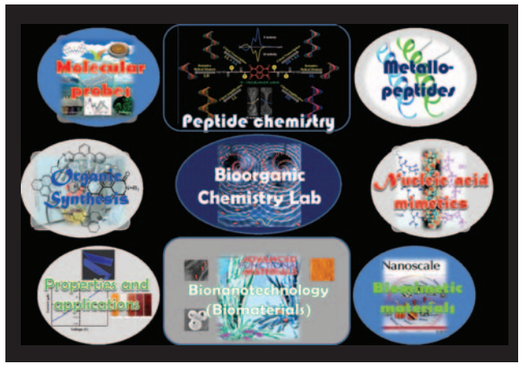
ORGANIC SYNTHESIS, MOLECULAR PROBES, PEPTIDE AND PROTEIN CHEMISTRY, NUCLEIC ACID CHEMISTRY, BIONANOTECHNOLOGY

Our research activities are at the interface of chemistry, biology and materials. We actively pursue the design and synthesis of small molecules, peptides, nucleic acids and their conjugates based biomimetic systems and materials possessing well defined nano-, meso- and micro-structures with properties similar to natural materials through Nature-inspired molecular self-assembly approach. These biomimetic materials find applications as biomaterials, drug delivery systems, composites and in bioelectronics. We are also involved in developing chiral unnatural amino acids and ligands for molecular recognition and sensing applications through supramolecular host-guest interactions. We are undertaking the design and synthesis of new class of smart-building blocks for metal directed assemblies for biosensors and smart materials applications. In our laboratory protocols have been established to develop biomimetic molecular self-assembly-based systems and materials through chiral transcription, amplication and retentive helical memory for use in chiral technology (separation, catalysis etc) and to understand spontaneous deracemization and amplication pathways for biological homochirality.



KEY PUBLICATIONS

M. B. Avinash and T. Govindaraju, *Engineering molecular organization of naphthalenediimides: large nanosheets with metallic-conductivity and attoliter containers,* **Advanced Functional Materials 2011. 20,** 3875-3882.

M. B. Avinash and T. Govindaraju, *A bio-inspired design strategy: Organization of tryptophan-appended naphthalenediimide into well-defined architectures induced by molecular interactions,* **Nanoscale 2011, 3,** 2536-2543.

T. Govindaraju, M. Pandeeswar, G. Jaipuria and H. S. Atreya, *Spontaneous self-assembly of designed cyclic dipeptide (Phg-Phg) into two-dimensional nano- and mesosheets,* **Supramolecular Chemistry 2011, 23,** 487-492.

D. Maity, A. K. Manna, D. Karthigeyan, T. K. Kundu, S. K. Pati, and T. Govindaraju, *Visible-near infrared and fluorescent copper sensors based on julolidine conjugates: selective detection and fluorescence imaging in living cells,* **Chemistry-A European Journal 2011. 17,** 11152-11161.

D. Maity and T. Govindaraju, *Pyrrolidine constrained bipyridyl-dansyl click fluoroionophores as selective Al(III) sensor,* **Chemical Communications 2010, 46,** 4499-4501.

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BIO-ORGANIC AND MEDICINAL CHEMISTRY

Infectious diseases remain a major threat to global health, and are now the world's biggest killers, causing over 15 million deaths per year. The threat is compounded by the fact that an increasing percentage of pathogens are developing resistance to the available arsenal of drugs. Therefore, there is an urgent need for a well-coordinated and integrated approach to tackle the threat of infectious diseases.

Our laboratory seeks to provide a platform to integrate organic chemistry and material science with biology to combat infectious diseases in a multipronged approach, namely, diagnosis, prevention and treatment. Our research focuses on the fundamental understanding of material-pathogen interaction, and development of innovative strategies that will provide solutions in tackling infections. We are involved in creating novel antimicrobial agents for the prevention and treatment of infectious diseases and combating the emergence of antimicrobial resistance. Additionally, we are interested in developing nanotechnology-based smart drug delivery systems for addressing nonspecific action and toxicity-related issues of existing drugs, for indications like infectious diseases and cancer.

Our specific research interests are Antimicrobial Therapeutics, Antimicrobial and Antifouling Materials, and Smart Drug Delivery Systems.

KEY PUBLICATIONS

J Hoque, P Akkapeddi, V Yarlagadda, DSSM Uppu, P Kumar, and J Haldar, *Cleavable Cationic Antibacterial Amphiphiles: Synthesis, Mechanism of Action, and Cytotoxicities,* **Langmuir 28,** 12225 (2012).

J Hoque, P Kumar, VK Aswal and J Haldar, *Aggregation Properties of Amide Bearing Cleavable Gemini Surfactants by Small Angle Neutron Scattering and Conductivity Studies,* **Journal of Physical Chemistry B 116,** 9718 (2012).

AK Weight, J Haldar, LA De Cienfuegos, LV Gubareva, TM Tumpey, J Chen, and AM Klibanov, *Attaching zanamivir to a polymer markedly enhances its activity against drug-resistant strains of influenza A viruses,* **Journal of Pharmaceutical Sciences 100,** 831 (2011).

AM Larson, B Hsu, D Rautaray, J Haldar, J Chen, and AM Klibanov, *Hydrophobic polycationic coatings disinfect poliovirus and rotavirus solutions,* **Biotechnology and Bioengineering 108,** 720 (2011).

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DESIGNING NEW WAYS TO SMALL MOLECULE HETEROCYCLIC SCAFFOLDS

Small molecule heterocyclic ligands play an important role in drug discovery research, and can exert powerful effects on the function of the macrocycles that comprise living systems. For several years, our Group has been involved in the design and development of new, highly efficient, innovative general methods for thesynthesis of a large variety of structurally diverse and regiospecifically functionalized five- or six-membered heterocycles and their condensed analogs, which are structural components of a large number of pharmaceutical agents as pharmacophores of considerable importance.

Our diversity-oriented synthesis of these molecules relies upon the development of a new class of three carbon 1,3- electrophilic organosulfur building block precursor pool which are readily accessible in a one-pot reaction from a wide range of cheap, active methylene compounds. These newly discovered synthetic protocols are highly effective for heterocycle synthesis and the elaboration of diverse substitution patterns for complexity generation on heterocyclic frameworks. They are especially suitable in combinatorial chemistry for rapid generation of libraries of diverse combinatorial arrays for discovery, and optimization of new lead structures in drug discovery research.

Another area of our research interest revolves around the design and development of new complexity-generating, multistep one-pot reactions such as domino reactions and multicomponent reactions for accelerating the discovery process; the discovery of new reagents; and the total synthesis of biologically important natural products such as the cytotoxic compounds, Horsifiline, and Coerusuline, as well as the DNA Topoisomerase inhibitor, cryptotackiene. Most recently, we have been exploring transition metal catalyzed C-C and C-heteroatom bond forming reactions for construction of novel heterocyclic scaffolds.

KEY PUBLICATIONS

S Kumar, and H Ila, *Novel Routes to Pyrazolo[3,4-b]indoles and Pyrazolo[1,5-a]benzimidaoles via palladium and copper catalyzed Intramolecular C-C and C-N bond formation,* **Journal of Organic Chemistry 74,** 7046 (2009).

S Kumar, S Peruncheralathan, H Ila, and H Junjappa, *A Novel Anionic Domino Process for the Synthesis o-Cyanoaryl-Methylthio/ Alkyl/ Aryl/ Heteroaryl Acetylenes, Organic Letters 10, 965, (2008). NC Misra, K Panda, H Ila, and H Junjappa, An Efficient Highly Regioselective Synthesis of 2,3,4-Trisubstituted Pyrroles by Cycloaddition of Polarized Ketene S,S- and N,S- Acetals with Activated Methylene Isocyanides,* **Journal of Organic Chemistry 72,** 1246 (2007).

AK Yadav, S Peruncheralathan, H Ila, and H Junjappa, *Domino Carbocationic Rearrangement of a-[Bis(methylthio)methylene]alkyl-2-(3/2-indolyl) Cyclopropyl Ketones,* **Journal of Organic Chemistry 72,** 1388 (2007).

H Ila, H Junjappa, and PK Mohanta, *The Junjappa-Ila (JI)-Heteroaromatic Annulation: A New General α-Oxoketene Dithioacetals Mediated Inverse Method for the Synthesis of Benzo/Condensed Heterocycles and Related Heteroaromatization Processes,* **Progress in Heterocyclic Chemistry,** GW Gribble, TL Gilchrist, eds., Pergamon Press, Vol. 13, 1 (2001).

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INORGANIC AND SOLID STATE CHEMISTRY

Our Group is focused on solid state inorganic materials from exploratory synthesis in intermetallics, chalcogenides, and polyoxometallates. We have a wide range of facilities available in our lab for the synthesis of bulk compounds, as well as single crystal growth. We study phase purity, and establish the crystal structure, using X-ray diffraction on single crystals.

In intermetallics, our focus is mainly on rare earth systems which can exhibit interesting physical properties, such as the Kondo effect, valence fluctuation, heavy fermion, superconductivity, structural transitions, and zero thermal expansion. Our research on chalcogenide materials focuses on photovoltaic and non-linear optical applications, while our study of polyoxometallates is mainly its use as a catalyst for various organic reactions.

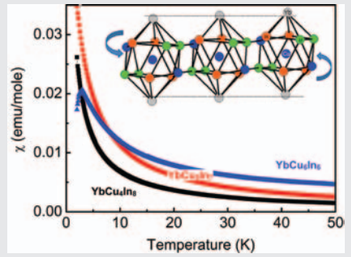

Fig. : Influence of structural distortion on the temperature dependent magnetic susceptibility of $YbCu_{6-x}In_{6+x}$ (x = 0, 1, 2). The distortions in the crystal structure are marked with arrows in the inset.

KEY PUBLICATIONS

Udumula Subbarao, and Sebastian C Peter, *Crystal Structure of $YbCu_6In_6$ and Mixed Valence Behavior of Yb in $YbCu_{6-x}In_{6+x}$ (x=0,1,2) Solid Solution,* **Inorganic Chemistry 51,** 6326 (2012).

Abhishek K Iyer, and Sebastian C Peter, *$EuLige_2$ and $YbLiGe_2$ - A divalent and an IntermediateValent Compound with $CaLiSi_2$- Type Structures,* **European Journal of Inorganic Chemistry,** 2012, 1790-1794.

Sebastian C Peter, Maria Chondroudi, Christos D Malliakas, Mahalingam Balasubramanian and Mercouri G Kanatzidis, *Anomalous Thermal expansion in the square-net compounds RE_4TGe_8(RE=Yb,Gd;T=Cr-Ni,Ag),* **Journal of the American Chemical Society 133,** 13840 (2011).

John Androulakis, Sebastian C Peter, Hao Li, Christos D Malliakas, John A Peters, Zhifu Liu, Bruce W Wessels, Jung--Hwan Song, Hosub Jun, Arthur J Freeman, and Maercouri G Kanatzidis, *Dimensional reduction: a design tool for new radiation detection materials,* **Advanced Materials 23,** 4163 (2011).

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UJJAL K GAUTAM OBTAINED HIS MASTERS AND Ph.D. DEGREES FROM THE INDIAN INSTITUTE OF TECHNOLOGY, DELHI, AND THE INDIAN INSTITUTE OF SCIENCE, BANGALORE, RESPECTIVELY. HE WORKED AS A POST-DOCTORAL FELLOW AT THE NATIONAL INSTITUTE FOR MATERIALS SCIENCE, TSUKUBA, JAPAN, BEFORE JOINING THE INTERNATIONAL CENTER FOR YOUNG SCIENTISTS AT THE SAME INSTITUTE, AS AN INDEPENDENT RESEARCHER. HE JOINED JNCASR IN 2011.

NANOMATERIALS AND RENEWABLE ENERGY

INORGANICALLY FILLED CARBON NANOTUBES

A new class of heterostructures, Carbon Nanotubes (CNT), provide the tiniest and unique storage space due to its opacity, and thermal and chemical stability. We have been creating nanostructures of metals, superconductors, oxides, sulfide and nitrides inside CNT.

PHOTOCATALYTIC WATER SPLITTING FOR RENEWABLE HYDROGEN ENERGY

Hydrogen can combine with oxygen to produce harmless water and a lot of energy, and therefore, can substitute the fast-depleting fossil fuels. While oxygen in available in the air, hydrogen has to be generated by splitting water. This can be achieved with the help of sunlight in the presence of catalysts. We are interested in the development of a new class of nanomaterial-based catalyst for this purpose.

SYNTHESIS OF MATERIALS AT THE LIQUID-LIQUID INTERFACE

The liquid-liquid interface is a non-homogeneous, two-dimensional confined space with a thickness of a few nanometers. The interfacial reactions differ due to reduced dimensionality, and partial distribution of the reactants in either of the phases. We are interested in alternative reaction mechanisms possible under these unusual conditions.

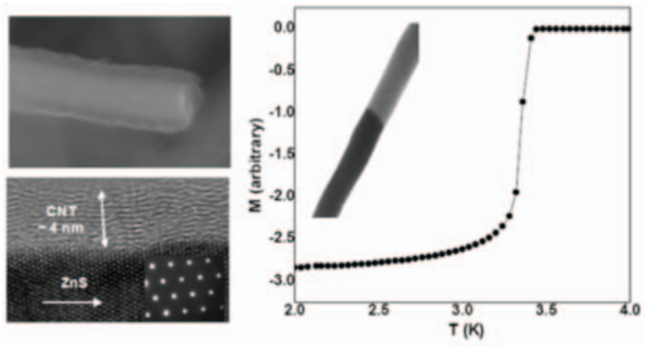

Fig. : Filled carbon nanotubes with single-crystalline materials. Some of the filled materials are exotic hetero-structures such as metal-Insulator or superconductor-semiconductors

KEY PUBLICATIONS

PMFJ Costa, UK Gautam, Y Bando, and D Golberg, *Direct imaging of Joule heating dynamics and temperature profiling inside a carbon nanotube interconnect,* **Nature Commun. 10,** 1038/ ncomms1429 (2011).

X Fang, T Zhai, UK Gautam, L Li, L Wu, Y Bando, and D Golberg, *ZnS nanostructures: From synthesis to applications,* **Prog. Mater. Sc. 56,** 175 (2011).

UK Gautam, M Imura, C Sekhar Rout, Y Bando, X Fang, B Dierre, L Sakharov, A Govindaraj, T Sekiguchi, D Golberg, and CNR Rao, *Unipolar assembly of zinc oxide rods manifesting polarity-driven collective luminescence,* **Proc. Natl. Acad. Sci. 107,** 13588 (2010).

Kanishka Biswas

KANISHKA BISWAS RECEIVED HIS Ph.D. AND MS IN CHEMISTRY FROM SSCU, INDIAN INSTITUTE OF SCIENCE, BANGALORE, INDIA AND WAS A POSTDOCTORAL FELLOW AT THE DEPARTMENT OF CHEMISTRY, NORTHWESTERN UNIVERSITY, USA, BEFORE JOINING THE NEW CHEMISTRY UNIT, JNCASR.

SOLID STATE INORGANIC CHEMISTRY

The research of our Group is focused on solid state inorganic chemistry of bulk/ nano-structured metal chalcogenides and thermoelectric property investigations. With about two-thirds of utilised energy being lost as waste heat, there is a compelling need for low-cost, environment-friendly, high performance thermoelectric materials that can directly and reversibly convert heat to electrical energy. Research in the area of alternative energy solutions such as thermoelectrics will open a new window to tackle the upcoming energy problems of the future. Thermoelectric research is based on the synthesis of bulk inorganic metal chalcogenides, the measurement of electronic charge and thermal transport properties, and the understanding of structure-property relationships. Apart from solid state chemistry, the research interest of the Group is also focused on soft-chemical solution phase synthesis, and growth and novel property studies (such as magnetic, thermoelectric, and catalytic) of inorganic metal chalcogenide nanoparticles and nanorods.

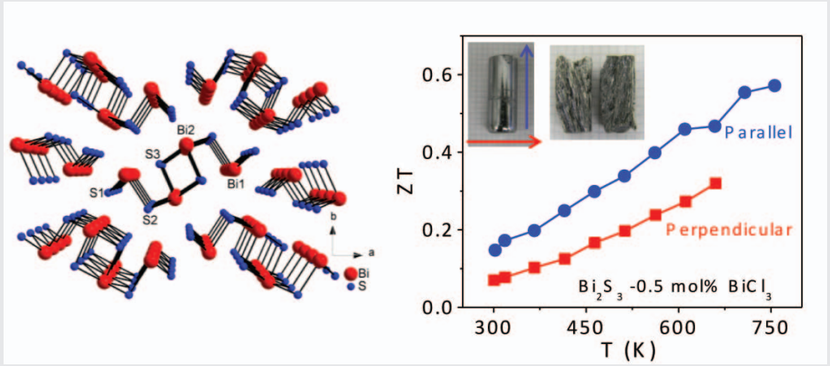

Fig.: Tellurium free thermoelectrics: the anisotropic n-type semiconductor Bi_2S_3.

KEY PUBLICATIONS

K Biswas, J He, Q Zhang, G Wang, C Uher, VP Dravid, and MG Kanatzidis, *Strained endotaxial nanostructure with high thermoelectric figure of merit,* **Nature Chem. 3,** 160 (2011).

K Biswas, J He, G Wang, S-H Lo, C Uher, VP Dravid, and MG Kanatzidis, *High thermoelectric figure of merit in nanostructured p-type PbTe-MTe (M = Ca, Ba),* **Energy Environ. Sci. 4,** 4675 (2011).

I Chung, K Biswas, JH Song, J Androulakis, K Chondroudis, KM Paraskevopoulos, AJ Freeman, and MG Kanatzidis, *$Rb_4Sn_5P_4Se_{20}$: A semi-metallic selenophosphate,* **Angew. Chem. Int. Ed. 50,** 8834 (2011).

K Biswas, Q Zhang, I Chung, JH Song, J Androulakis, AJ Freeman, and MG Kanatzidis, *Synthesis in ionic liquids: $[Bi_2Te_2Br](AlCl_4)$ a direct gap semiconductor with a cationic framework,* **J. Am. Chem. Soc. 132,** 14760 (2010).

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THEORETICAL SCIENCES UNIT

TSU

"It is the theory that decides what can be observed!", said Albert Einstein. Science without theory is unthinkable: theoreticians provide our fundamental understanding of how nature operates, and can also turn this knowledge into practical applications. In the Theoretical Sciences Unit at JNCASR, we aim to address, explain and understand the rich diversity we observe in the physical world, be it in the properties of materials, the way in which matter responds to external stimuli, or the modes of reproduction of living organisms. We also use this understanding for practical applications such as predicting new phenomena, or designing new materials. For this, we use the techniques of theoretical physics and chemistry. We are also interested in interdisciplinary areas, such as evolutionary biology, in which techniques and ideas from physics can be used to gain fresh insight.

The research in our Unit is inspired by two complementary approaches to the study of matter and life: the search for universality, and the exploration and explanation of diversity. In the very early universe, matter was homogoneous, but this is clearly no longer so. Due to "spontaneously broken symmetries" and sequences of phase transitions, the world around us now displays variety and complexity: carbon is ultrahard as diamond or soft as graphite, ice contracts when it melts whereas copper expands, chewing gum stretches when stepped on whereas glass shatters, and most of life is multicellular and sexually reproducing, though these are expensive traits... Why? In order to understand this fascinating yet perplexing range of behaviour, we have to examine structures and properties at a fundamental level, and consider the complex consequences of having a large number of entities (be they electrons, atoms, molecules or living creatures) that interact strongly with one another. One fascinating aspect is that even when the underlying natural laws are simple in form, complex behaviour can be manifested as system sizes increase.

Our faculty members have had their basic training in many body physics, computational chemistry, quantum mechanical density functional theory, statistical mechanics, and mathematical physics. However, much of the work we currently pursue is interdisciplinary in nature, so that we turn the boundaries between these fields into seamless ones. Accordingly, we also accept students who have undergraduate or graduate degrees in a variety of academic disciplines, such as chemistry, physics, engineering, and computer science.

In addition to collaborating amongst ourselves on various problems, we also interact with our experimental colleagues, both, in JNCASR, and outside. We use a mixture of analytical and computational techniques; in the latter, we are helped by the presence of high-performance computational facilities at JNCASR.

The atmosphere in our Unit is vibrant, informal and interactive. Our faculty and students participate in a number of national and international conferences and workshops. We organise several seminars and colloquia ourselves, and have a constant stream of distinguished visitors. Alumni of our Unit have excelled in their careers; several of them are now establishing their own groups at universities in India and abroad. We are always on the lookout for bright students who are curious about science and dedicated to research; we urge you to contact us if you are one of them!

RECENT Ph.D. & M.S. THESES (2011-2012)

- Diagrammatic Perturbation Theory based Investigations of the Mott Transition Physics (Himadri Barman, Ph.D., 2011)
- Understanding the Electronic Structure of Organometallic Sandwich Complexes and Graphene based Nanomaterials [Ershaad Ahamed Basheer, M.S.(Engg.), 2011]
- Mechanical Behavior of Ni-based Superalloys having γ/γ' Interface: A First-principles Study [Kaushlendra Kumar, M.S.(Engg.), 2011]
- Adaptation on Rugged Fitness Landscapes [Sarada S, MS(Engg.), 2011]
- Density Functional Theory Study of Structural and Magnetic Properties of Low Dimensional Systems (Mighfar Imam, Ph.D., 2012)
- Methods and Models for the Study of Structure, Cold Denaturation and Aggregation of Proteins (Moumita Maiti, Ph.D., 2012)

CITATION/AWARDS

Subir Das: Regular Associateship of International Centre for Theoretical Physics, Trieste, Italy, 2010.

Shobhana Narasimhan: Kalpana Chawla Award of the Government of Karnataka, 2010.

Swapan Pati: "Shanti Swarup Bhatnagar Prize" Awarded by CSIR in Chemical Sciences, 2010.

CITATION/AWARDS

Umesh Waghmare: "Shanti Swarup Bhatnagar Prize" Awarded by CSIR in Physical Sciences, 2010.

Vidhyadhiraja NS: Adjunct Associate Research Professor at the Birck Nanotechnology Centre, Purdue University (Jun 2011 - May 2014).

Umesh V Waghmare

UMESH WAGHMARE RECEIVED A BTech (WITH THE INSTITUTE SILVER MEDAL) IN ENGINEERING PHYSICS FROM THE INDIAN INSTITUTE OF TECHNOLOGY, BOMBAY, AND A Ph.D. IN APPLIED PHYSICS FROM YALE UNIVERSITY. HE WORKED AS A POST-DOCTORAL RESEARCH ASSOCIATE IN THE PHYSICS DEPARTMENT AT HARVARD UNIVERSITY BEFORE JOINING JNCASR IN 2000.

MATERIALS THEORY GROUP

Professor Waghmare's work involves connecting first-principles quantum mechanical description of materials with their behavior at various time and length-scales. To achieve this challenging task of linking microscopic structure and chemistry of a material to its macroscopic properties, they typically develop a model Hamiltonian by integrating out high-energy of degrees of freedom and retaining only those relevant to the essential physics of the material. This procedure involves effective use of symmetries (Group theory) and basic principles of statistical mechanics. The resulting effective Hamiltonian models are realistic, yet tractable, and are used in quantitative prediction of material-specific properties at various length and time scales as a function of temperature.

As first-principles theory of materials assumes no empirical inputs, it not only complements experiments by accessing information at the atomic scale, but also has the ability to predict novel materials and structures ahead of experiments. Prof. Waghmare's work has led to prediction of lead-free ferroelectrics and novel line defects in graphene, both of which were later verified experimentally. One of the recent accomplishments of the group is the development of a generalized Ginzburg-Landau theory of ferroelectrics from first-principles.

The Materials Theory Group is presently investigating the following areas:
Multifunctional smart materials, which include ferroelectrics, multiferroics, magnetic semiconductors, shape-memory alloys.

Nanomaterials, with current focus on nanotubes and 2-dimensional nanomaterials such as graphene, BN, BCN, MoS_2, $MoSe_2$, and physics of defects in these materials.

Mechanical behaviour of materials, physics of grain boundaries, stacking faults and crack propagation, particularly in Ni-Al superalloys and Ti-alloys.

Materials for energy and environment, including thermoelectrics, materials for hydrogen storage, photoelectrocatalytic splitting of water, materials for electrodes in Li-ion batteries, and catalysts for oxidation of CO and NO.

KEY PUBLICATIONS

KS Subrahmanyam, P Kumar, U Maitra, A Govindaraj, KPSS Hembram, UV Waghmare, and CNR Rao, *Chemical Storage of Hydrogen in Few Layer Graphene,* **Proceedings of National Academy of Sciences of the United States of America 108,** 2674 (2011).

Anil Kumar, and UV Waghmare, *First-principles free energies and Ginzburg-Landau theory of domains and ferroelectric phase transitions in* $BaTiO_3$, **Physical Review B 82,** 054117, (2010).

Nirat Ray, and UV Waghmare, *Coupling between magnetic ordering and structural instabilities in perovskite biferroics: A first-principles study,* **Physical Review B 77,** 134112 (2008).

J Paul, T Nishimatsu, Y Kawazoe, and UV Waghmare, *Ferroelectric phase transitions in ultrathin films of* $BaTiO_3$, **Physical Review Letters 99,** 077601 (2007).

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STATISTICAL PHYSICS OF EQUILIBRIUM AND NON-EQUILIBRIUM CONDENSED MATTER SYSTEMS

My Group is interested in condensed matter systems, both at and away from equilibrium, to understand which we use analytical and numerical techniques of statistical mechanics. In this broad area, our recent focus has been in Phase Transition and Critical Phenomena, Kinetics of Phase Separation in Multicomponent Mixtures, Structure and Dynamics in Confined Systems, Pattern Formation, Nucleation, and Wetting. We investigate universality in both static and dynamic properties occurring in apparently different systems.

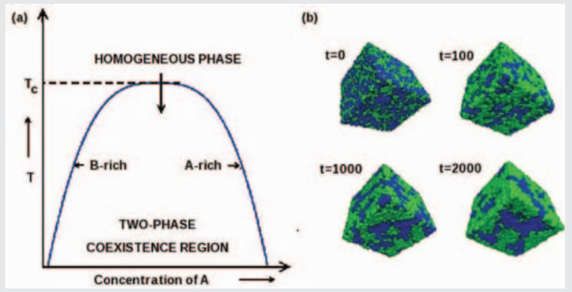


Fig. 1: (a) Phase diagram of a symmetric binary (A+ B) mixture. (b) Pattern formation during phase separation when a homogeneously mixed (t=0) 50:50 binary fluid is quenched below the critical temperature, Tc

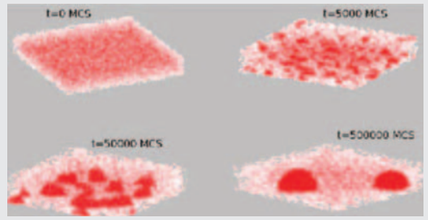


Fig. 2: Nucleation and growth of droplets on a wall of a thin film of solid binary mixture with offcritical composition

KEY PUBLICATIONS

SK Das, **Europhysics Letters EPL 97,** 46006 (2012).

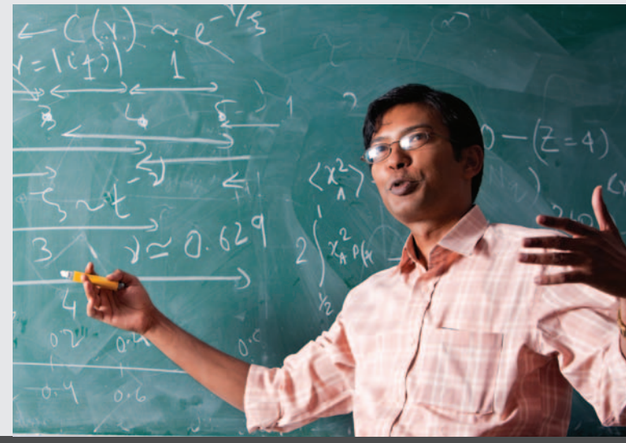
S Roy, and SK Das, **Europhysics Letters EPL 94,** 36001 (2011).

S Majumder, and SK Das, **Europhysics Letters EPL 95,** 46002 (2011).

SK Das, YC Kim, and ME Fisher, **Physical Review Letters 107,** 215701 (2011).

SK Das, and K Binder, **Physical Review Letters 107,** 235702 (2011).

S Majumder, and SK Das, **Rapid Communication Physical Review E 81,** 050102 (2010).



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KAVITA JAIN RECEIVED HER Ph.D. FROM TATA INSTITUTE OF FUNDAMENTAL RESEARCH, MUMBAI, AND PURSUED HER POST-DOCTORAL RESEARCH AT THE UNIVERSITY OF COLOGNE, GERMANY, AND THE WEIZMANN INSTITUTE OF SCIENCE, ISRAEL. SHE HAS BEEN WITH JNCASR SINCE 2007.

MATHEMATICAL MODELS OF BIOLOGICAL EVOLUTION

We are interested in statistical physics and probability theory, and their applications to interdisciplinary areas such as biological evolution. We address questions in these fields using analytical calculations and numerical simulations.

Our research in biological evolution involves modeling experimental situations and predicting new biological phenomena which can be tested experimentally. With this goal in mind, we have studied population genetics models of punctuated evolution, predictability of evolutionary trajectories, evolution of sex and evolution of mutation rates.

Our recent work has focused on the evolution of large deterministic populations on correlated fitness landscapes, and the adaptation dynamics of stochastically evolving populations on rugged fitness landscapes which can get trapped at a local fitness peak.

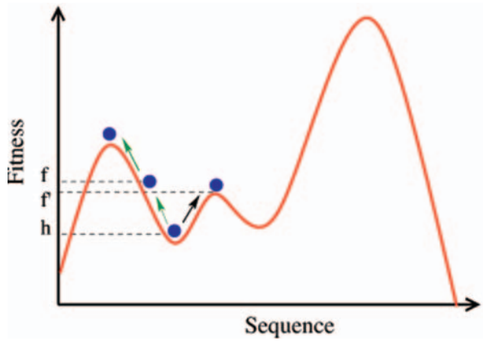

Fig. : Schematic diagram to illustrate adaptive walk on a rugged fitness landscape with many local maxima. The population (filled circle) with fitness h has fitter one- mutant neighbors with fitness f,f',..., one of which is chosen with a certain transition probability. The global maximum is not accessible to the population as it is not a one- mutant neighbor and the walk terminates when the population reaches a local fitness maximum

KEY PUBLICATIONS

Kavita Jain, Joachim Krug, and Su-Chan Park, *Evolutionary advantage of small populations on complex fitness landscapes,* **Evolution 65,** 1945 (2011).

Kavita Jain, and Sarada Seetharaman, *Multiple adaptive substitutions during evolution in novel environments,* **Genetics 189,** 1029 (2011).

Kavita Jain, *Time to fixation in the presence of recombination,* **Theoretical Population Biology 77,** 23 (2010).

Sarada Seetharaman, and Kavita Jain, *Evolutionary dynamics on strongly correlated fitness landscapes,* **Physical Review E 82,** 031109 (2010).

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SHOBHANA NARASIMHAN HAS A Ph.D. IN PHYSICS FROM HARVARD UNIVERSITY. SHE WAS A POST-DOC AT BROOKHAVEN NATIONAL LABORATORY, AND THE FRITZ-HABER-INSTITUT, BERLIN, AND HAS HELD VISITING POSITIONS AT THE UNIVERSITY OF CAMBRIDGE, THE UNIVERSITY OF PARIS, AND THE MAX PLANCK INSTITUT, STUTTGART.

NOVEL PHYSICS AND CHEMISTRY AT THE NANOSCALE

In my Group, we use theoretical and computational techniques to examine how structural, mechanical, electronic, magnetic, and chemical properties change at the nanoscale. Some of the problems we work on have technological relevance for pressing problems such as clean energy and device miniaturization. The main tool we use is quantum mechanical density functional theory. Such *ab initio* calculations require no empirical input, other than atomic numbers and masses.

MIXING ON SURFACES

From ancient times, it has been known that mixing two or more metals to form an alloy can result in a material with superior properties. Unfortunately, many combinations of metals do not form alloys in the three-dimensional bulk. However, could such metals form alloys when confined to a single atomic layer at the surface? Together with our experimental collaborators, we have identified many such systems. One of these is FeAu2/Ru(0001), a long-range ordered surface alloy, which, our calculations show, is stabilized by magnetic interactions.

NANOMAGNETISM

Many magnetic materials become “more magnetic” at small sizes, and some non-magnetic materials become magnetic in the nanodomain. These are only some of the fascinating aspects of magnetism at the nanoscale. One quantity of particular interest to us is the magnetic anisotropy energy, which is the energy required to flip a spin. This is what matters if one wants to ensure that thermal fluctuations don’t destroy data that has been stored magnetically. We also look at novel magnetic structures such as spin spirals.

THE ‘RATIONAL DESIGN’ OF CATALYSTS

Much of modern life would be unthinkable without catalysts, for instance, catalytic converters are necessary to clean up noxious products in automobile exhaust. The surprising thing is that most currently used catalysts were developed by a process of trial and error. We are a part of the worldwide effort to replace this by rational design guided by quantum mechanical calculations. One example of a problem we have been looking at recently is tailoring nanocatalyst shapes (and hence catalytic properties) by doping the oxide substrates on which the nanoparticles are deposited.

SPINTRONICS

Can one use the electron spin instead of the charge for an alternative or supplement to electronics? We are exploring this new frontier area through transport calculations where we place molecules between magnetic leads.

OTHER AREAS

Natural gas storage in the form of gas cylinders is both cumbersome and unsafe. We have worked on strategies for increasing the absorption of methane in activated carbons, which are a cheap and versatile storage medium. To do this, we have studied defective and chemically functionalized graphene as a model system.

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Swapan Kumar Pati

SWAPAN KUMAR PATI GOT HIS Ph.D. IN SOLID STATE AND STRUCTURAL CHEMISTRY FROM THE INDIAN INSTITUTE OF SCIENCE, BANGALORE. HE THEN DID TWO POST-DOCTORAL RESEARCHES, ONE IN PHYSICS AT THE UNIVERSITY OF CALIFORNIA, DAVIS AND THE SECOND ONE IN CHEMISTRY, AT NORTHWESTERN UNIVERSITY, EVANSTON, USA. HE JOINED JNCASR IN 2000, AND HIS MANY AWARDS AND HONOURS INCLUDE FELLOWSHIP OF TWO INDIAN ACADEMIES AND THE SHANTI SWARUP BHATNAGAR AWARD IN CHEMICAL SCIENCES.

CHEMISTRY AND PHYSICS OF SYSTEMS RANGING FROM ATOMS TO EXTENDED MATERIALS

The focus of research of Dr. Pati's group has been to understand the structure property relationships of a large class of systems, ranging from simple molecules to polymeric materials, where quantum effects give rise to many exotic phenomena. The goal is to design and model materials for microscopic understanding and applications purposes.

The current areas of interest of the Group are: Quantum Magnetism, Electrical Transport through Molecules/ Dots, Nano-materials and New Carbon systems, Cold atom phenomena, Generalized Charge transfer and Quantum Kinetics in biological and bio-mimetic systems, Development of novel methods for studying diverse response phenomena arising from excited states.

KEY PUBLICATIONS

Graphene and Its Fascinating Attributes, ed. Swapan K Pati, Toshiaki Enoki, and CNR Rao, Singapore: World Scientific Publishing (2011),ISBN: 978-981-4329-35-4.

Dibyajyoti Ghosh, Ganga Periyasamy, and Swapan K Pati, *Density Functional Theoretical investigation of the aromatic nature of the BN substituted Benzene and four ring polyaromatic hydrocarbons,* **Physical Chemistry Chemical Physics 13,** 20627 (2011).

Debabrata Maity, Arun K Manna, D Karthigeyan, Tapas K Kundu, Swapan K Pati, and T Govindaraju, *Visible-near infrared and fluorescent copper sensors based on julolidine conjugates: selective detection and fluorescence imaging in living cells,* **Chemistry: A European Journal 17,** 11152 (2011).

Arun K Manna, and Swapan K Pati, *Tunable Electronic and Magnetic Properties in BxNyCz Nanohybrids: Effect of Domain Segregation,* **Journal of Physical Chemistry C 115,** 10842 (2011).

Ershaad Ahmed Basheer, Prakash Parida, and Swapan K Pati, *Electronic and magnetic properties of BNC nanoribbons: a detailed computational study,* **New Journal of Physics 13,** 53008 (2011).

Prakash Parida, Swapan K Pati, and A Painelli, *Negative Differential Conductance in Nano-junctions: A Current Constraint Approach,* **Physical Review B 83,** 165404 (2011).

Arun K Manna, and Swapan K Pati, *Doping single-walled carbon nanotubes through molecular charge-transfer: a theoretical study,* **Nanoscale 2,** 1190 (2010).

Sudipta Dutta, and Swapan K Pati, *Novel Properties of Graphene Nanoribbons: A Review,* **Journal of Materials Chemistry 20,** 8207 (2010).

Sairam S Mallajosyula, and Swapan K Pati, *Towards DNA Conductivity : A Theoretical Perspective (A Review),* **Journal of Physical Chemistry Letters 1,** 1881 (2010).

Sudipta Dutta, and Swapan K Pati, *Edge reconstructions induces magnetic and metallic behavior in zigzag graphene nanoribbons,* **Carbon 48,** 4409 (2010).

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PHASE TRANSFORMATIONS AND DYNAMICS IN SOFT CONDENSED MATTER, AND BIOLOGICAL SYSTEMS

My Group's research is in the area of statistical mechanics, with a focus on understanding a range of unusual and interesting properties of liquids and other disordered – typically fluid – substances, described generally as soft condensed matter. Entropy plays a large role in determining the properties of these systems, and thermal effects are important. Such systems can exhibit rich phase behavior, complex microscopic dynamics, response to external perturbation, and related time-dependent phenomena. Inclusion of metastable states extends the time-dependent phenomena of interest to the kinetics of phase transformations. Finally, understanding the full range of possible (history-dependent) fates of such systems requires understanding of routes to structural arrest, exemplified by glass formation in dense liquids. The properties and phenomena mentioned here form the scope of our research.

The approach in studying these properties and phenomena has typically been to understand them on the basis of a microscopic description that is sufficiently detailed to describe specific classes of systems, rather than to study highly idealized models or to attempt extremely accurate representations. Computation emerges naturally as a relevant tool, and has been used extensively. Occasional investigations have also concerned more realistic or idealized models, and the use of other theoretical methods. In addition to using computational methods for research on problems of interest, we have an interest in the methodological aspects of effective computational study of condensed matter systems.

Some examples of ongoing work include the study of length scales associated with time scales of relaxation in glass forming liquids, modeling gelation, jamming, understanding glass forming ability, the study of a novel liquid-liquid phase transition in silicon, including the critical end point of the transition, the nature of the two liquid phases, and the role of liquid structure and critical fluctuations on rates of crystal nucleation. We also apply the ideas and methods developed in the above studies to the study of biomolecular systems, which have more complex molecular detail. Work along these lines includes the geometric analysis of protein structure, the protein glass transition and simple models for understanding protein aggregation.

KEY PUBLICATIONS

Moumita Maiti et al, *Potential of mean force between hydrophobic solutes in the Jagla model of water and implications for cold denaturation of proteins,* **J. Chem. Phys. 136,** 44512 (2012).

Shiladitya Sengupta et al, *Dependence of the fragility of a glass former on the softness of interparticle interactions,* **J. Chem. Phys. 135.** 194503 (2011).

Vishwas V Vasisht, Shibu Saw, and Srikanth Sastry, *Liquid-liquid critical point in supercooled silicon,* **Nature Physics 7,** 549 (2011).

Smarajit Karmakar, Chandan Dasgupta, and Srikanth Sastry, *Analysis of Dynamic Heterogeneity in a Glass Former from the Spatial Correlations of Mobility,* **Phys. Rev. Lett. 105,** 015701 (2010).

Shibu Saw, Niels L Ellegaard, Walter Kob, and Srikanth Sastry, *Structural relaxation of a Gel Modeled by Three Body Interactions,* **Phys. Rev. Lett. 103,** 248305-248308 (2009).

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NON-COMMUTATIVE PROBABILITY AND GEOMETRY: MATHEMATICS OF QUANTUM MECHANICS

The foundation of Quantum Mechanics has brought with it many new challenges to the mathematical community. It represents a whole new way of looking at spaces and functions as well as of assigning probabilities to hitherto non-compatible events, which is a truly non-Kolmogoroffian scenario.

One model of Non-commutative or Quantum Probability Theory was largely developed in the Delhi centre of the Indian Statistical Institute during the last two and a half decades. Besides being a new non-classical theory of probability and stochastic processes, it also provides a possible non-Hamiltonian model of quantum mechanical non-equilibrium systems. In this theory, the study of the structure of a semigroup of completely positive maps on the algebra of quantum observables and their stochastic dilations plays a crucial role.

Taking a hint from the fact that many topological and geometric properties of a classical space can be encoded into specific properties of the commutative algebra of functions of the space, one studies just these properties on a more general class of abstract topological or von Neumann algebras. Here, as well, intuition from Quantum Mechanics or Quantum Field Theory plays a crucial role.

Another area of contemporary research interest has been that of extending Krein's trace formula to multi-variable operator analysis. This is likely to have an impact on the computation of cyclic cohomology in non-commutative geometry.

KEY PUBLICATIONS

Kalyan B Sinha, *Data Matrices, Entropy and Applications (Dr. Rajendra Prasad Memorial Lecture delivered for the 64th ISAS conference in December 2010),* **Jour. Indian Soc. of Agri. Statistics, 65 (1),** 1-6 (2011).

Kalyan B Sinha, *Index theorems in Quantum Mechanics,* **Maths Newsletter, Special ICM 2010 Issue 19(1),** 195-203 (2010).

Kalyan B Sinha, Lingaraj Sahu, and Un Cig Ji, *Characterization of Unitary Processes with Independent increments,* **Comm. Stoch. Anal. 4(4),** 593-614 (2010).

Kalyan B Sinha, and Lingaraj Sahu, *Unitary processes with stationery increments,* **Ann. Inst. Henri Poincare Prob. Statistics 46(2),** 575-593 (2010).

Kalyan B Sinha, co-ed., **Advances in Math. Phys., Nonlinear and Non commutative Mathematics. New Developments and Applications in Quantum Physics,** Hindawi Publ. Corpn. (2010).

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CORRELATED ELECTRON SYSTEMS AND ORGANIC ELECTRONICS

Materials for which a single-particle description of electronic properties fails, are classified as correlated electron systems. Interest in these materials derives from the wide range of phenomena they exhibit such as high temperature superconductivity in cuprates, heavy fermions in lanthanides/ actinides, colossal magnetoresistance in manganites, and metal-insulator transitions in transition metal oxides. In recent years, there has been a resurgence of technological interest in these materials, which stems from the extraordinary sensitivity of transport and thermodynamic properties in these materials to external parameters such as temperature and pressure. Despite the decades of research in this area, enormous challenges remain for theoreticians and experimentalists.

Our Group employs diagrammatic perturbation theory-based techniques of Quantum Many Body Theory to understand these materials in the framework of simple models – the focus being to address issues relating to transport and thermodynamics, especially of heavy fermion systems and transition metal oxides.

Electronic devices based on organic polymers are emerging as inexpensive and efficient alternatives to traditional inorganic semiconductor based devices. Modeling of such devices is challenging because of the inherent strong disorder in polymer thin films. We have developed discrete circuit level approaches as well as kinetic Monte Carlo-based simulations for investigating charge transport and device modeling. This work is being carried out in close collaboration with the Molecular Electronics lab in JNCASR.

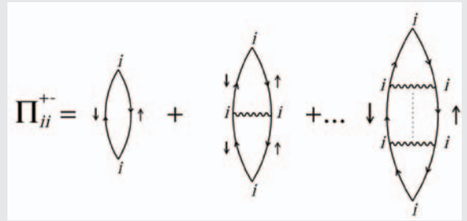

Fig. : Diagrammatic representation of the RPA for the transverse spin polarization propagator

KEY PUBLICATIONS

Pramod Kumar, and NS Vidhyadhiraja, *From mixed valence to the Kondo lattice,* **Journal of Physics: Condensed Matter 23,** 485601 (2011).

Himadri Barman, and NS Vidhyadhiraja, *Transport and spectra in the half-filled Hubbard model: a dynamical mean field study,* **Int. Journal of Modern Physics B 25,** 2461 (2011).

Dhritiman Gupta, NS Vidhyadhiraja, and KS Narayan, *Transport of Photogenerated Charge Carriers in Polymer Semiconductors,* **Proceedings of the IEEE 97,** 1558-1569 (2009).

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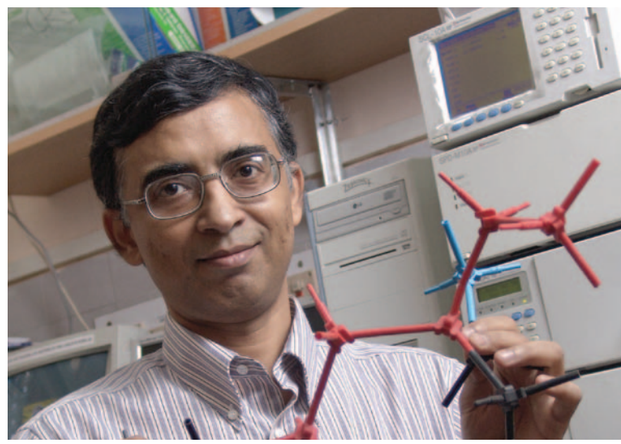
CHEMICAL BIOLOGY UNIT

The Chemical Biology Unit is a virtual Unit located on the campus of the Indian Institute of Science. The work carried out in this unit by the Honorary Faculty Members of JNCASR covers many of the emerging areas of chemical biology.

A significant segment of work in the Bhattacharya lab concentrates on the lipid molecular design, formation of membranous structure and assembly and uses them for gene transfection and related cellular delivery issues. Wide varieties of synthetic, spectroscopic, calorimetric, biochemical, molecular biological and computational tools are used to obtain information on the structure, stability and dynamics of various assemblies, lipoplexes and complexes that are formed. A corollary to the design of amphiphilic lipid molecules is the preparation of a large number of low molecular mass precursors, a few of which also manifest interesting aggregation properties, including the propensity of developing into two-dimensional 'films' and solvent entrapped 'gel', an interesting class of soft matter. The lab is attempting to understand the molecular basis of such phenomena, their flow behavior, temperature sensitivity and other attributes so that one can use them for specific biological or materials applications. Another focus of research involves molecular design of small molecule ligands that stabilize duplex, triplex and quadruplex DNA or even certain folds of RNA structures and exploit such properties for developing lead inhibitors for enzymes such as telomerase or topoisomerase etc.

The Balaram group has recently explored structure function studies of triosephosphate isomerase, a glycolytic enzyme, using Plasmodium falciparum and Methanocaldococcus jannaschii as models. Kinetic analysis of site specific mutants provides evidence for the involvement of Glu97 in the catalytic mechanism. The role of near active side residues in modulating the enzyme activity has also been explored. The enzyme from Drosophila Melanoglaster has been cloned and expressed as a model system to examine the relationship between disease causing human mutants and the activity. This group is also exploring structural studies of complex bioactive peptides isolated from natural sources.

Work in the Varadarajan lab is in the general area of protein structure and folding. A wide variety of spectroscopic, calorimetric, crystallographic, molecular biological and computational tools are used to obtain information on protein structure, stability and dynamics. The lab is interested in rationally modulating protein stability through mutation, understanding residue specific contributions to protein stability, improving methods for disulfide design and developing screens for identifying stabilized mutants of proteins. New methods for the design of temperature sensitive mutants of globular proteins have been developed. The



lab is attempting to understand the molecular basis for temperature sensitivity and has applied this understanding to rationally design temperature sensitive mutants in diverse organisms such as bacteria, yeast and fruitflies. Another focus of research is to produce stable, well folded molecules of HIV gp120/ gp41 immunogens for eventual use as part of an AIDS vaccine as well the design of inhibitors of viral entry into the cell. Similar approaches are also being used to design immunogens intended to produce neutralizing antibodies against influenza virus, another re-emerging global health threat.

The Maitra group is involved in the chemistry of bile acids. The studies of novel analogues of bile salts have led to the design of unusual gelators with potential applications. Thus, such bile gels have been used for the design of thermochromic materials, as templates for the design of inorganic nano structures, and also for the anchoring stabilized metal nanoparticles. Cationic analogues of bile acids have been extensively investigated by SANS and rheological measurements to understand their aggregation and flow properties. The current emphasis is on the development of functional or 'smart' gels. To this end, hybrid organic-inorganic soft materials have been created in which a lanthanide ion (typically europium or terbium, or a mixture of the two) can be used as luminescent handles. The first example of a self-assembled luminescent gel involving a sensitizer and a lanthanide were recently reported. This work has also led to the design of novel enzyme sensors using a 'pro-senitizer' strategy.

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CONDENSED MATTER THEORY UNIT

This Unit receives support from JNCASR in the form of funds for Research Associates, R&D assistants and Visitors, Computational Facilities and a contingency grant for day-to-day expenses and domestic travel.

The members of the CMTU are engaged in theoretical research on a variety of topics in the general area of Physics and Chemistry of Condensed Matter systems such as:

ELECTRONIC STRUCTURE, ESPECIALLY STRONGLY CORRELATED ELECTRON SYSTEMS

Dynamical effective medium theories; d-wave superconductivity in cuprates; strong correlation effects in systems of ultra cold atoms in optical lattices; Luttinger liquids and quantum wires; Molecular Magnetism and Photomagnetism; Electron-hole recombination, Triplet-triplet Annihilation and Excitation Transfer in Organic Light Emitting Diodes; Calculation of Auger spectra including matrix element effects; Calculation of X-ray magnetic circular dichroism spectra from compounds; Kinetically-driven magnetism in a class of magnetic compounds (double perovskites, dilute magnetic semiconductors); Studies of models of double perovskites; Electronic structure of semiconducting nanomaterials by real space calculations; Study of a spintronic material, Mn-doped GaAs, in the nanometric size regime; Theories of doped manganites, including spin, charge and orbital ordering effects; Studies of low-dimensional interacting quantum systems using the density-matrix renormalization group and other numerical methods.

EQUILIBRIUM AND NON-EQUILIBRIUM STATISTICAL MECHANICS OF SOFT CONDENSED MATTER AND OTHER COMPLEX SYSTEMS

Systems of vortex lines in high-Tc superconductors in the presence of pinning; Frustrated magnetic systems; Study of Portevin-Le Chatelier effect through time series analysis and modeling; Study of martensitic transformations; Multiscaling in fluid and magnetohydrodynamic turbulence; Spatiotemporal chaos and spiral turbulence in excitable media, including models for ventricular fibrillation; Semiflexible polymers; Dynamic scaling in driven systems; Orientational and solvation dynamics in complex liquids; Phase diagrams and dynamics of charged micellar systems; Dynamics of ions in complex porous networks and biomembranes; Numerical studies of the glass transition and slow dynamics in models of simple liquids; Equilibrium properties of classical fluids in a random potential; Complex networks in chemical, biological and social systems; Evolution of complexity in adaptive systems; Analytic and numerical studies of neural network models; Modeling of the growth of thin films under chemical vapour deposition and molecular beam epitaxy; The statistical mechanics of sedimentation; Dynamics and rheological chaos in surfactant solutions; Theory and experiments on ordered nonequilibrium steady states in agitated monolayers of granular rods; Statistical hydrodynamics of self-propelled organisms, from fish to bacteria to cell-membranes coupled to motors, filaments, and ATP; Rheology of the living cell.

RESEARCH FACILITIES

Network of workstations, personal computers and peripherals.

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HONORARY ASSOCIATE PROFESSOR

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CSIR CENTRE OF EXCELLENCE IN CHEMISTRY

• In January 1991, the CSIR established this person-based Centre of Excellence in Chemistry. The Centre works on various aspects of solid state and materials chemistry. The main activities of this CSIR-Centre deal with the following aspects.

• Developing new strategies for the synthesis, purification, functionalization and solubilization of novel carbon nanostructures such as, nanotubes (single-walled, double-walled and multi-walled), Y-junction nanotubes, metallic nanotubes, separation of metallic and semiconducting nanotubes from the mixture in a simple method to study the electrical transport, optical and other confinement properties. Synthesis of graphene nanoribbons by laser unzipping of nanotubes.

• Graphene is one of the main areas of research in this laboratory. Synthesis of two to four layer graphene by arc-discharge of graphite in a hydrogen atmosphere. Besides providing clean graphene surfaces, this method allows for doping with boron and nitrogen. UV and laser irradiation of graphene oxide provides fairly good graphene samples, Raman spectroscopy is used to investigate the charge-transfer interactions of graphene with electron-donor and -acceptor molecules, as well as with nanoparticles of noble metals. Notable potential applications of the properties of graphene are low turn-on field emission and radiation detection. High temperature ferromagnetism is another intriguing feature of graphene. Incorporation of graphene improves the mechanical properties of polymers, its incorporation with nanodiamond or carbon nanotubes exhibits extraordinary synergy.

• After the synthesis and characterization of graphene, serious attention is paid to other inorganic analogues of graphene. We have developed various chemical methods for the synthesis of layered transition metal dichalcogendes which includes MoS_2, WS_2, $MoSe_2$, WSe_2, NbS_2 and $NbSe_2$. We are studying their applications in IR detectors, gas sensors, composites with polymers for mechanical properties and electrical properties, magnetic properties, and hydro-desulphurization (HDS) catalysis. We have also used micromechanical cleavage method for obtaining the single-layers of MoS_2, GaS and GaSe and studied their applications in transistors, detectors and sensors.

• New method of synthesizing borocarbonitrides with significant surface area from low cost starting materials like urea, boric acid and activated charcoal has been discovered. Graphene-like $B_xC_yN_z$ samples with compositions close to BC_2N exhibit surface areas in the range 1500-1990 m^2/g, with the uptake values of CO_2 and CH_4 being in the ranges 97-128 wt % (at 195 K, 1 atm) and 7.5-17.3 wt % respectively. The CO_2 uptake in the case of the best BC_2N sample was 64 wt % at 298 K. The borocarbonitride samples show high uptake as well as selectivity of CO_2 over N_2. The adsorptive characteristics of borocarbonitrides are comparable to or better than those of some of the MOFs and other adsorbents reported in the recent literature. We have also prepared BC_xN where x varies between 1 and 2, by gas phase reaction of BBr_3 with ethylene and ammonia having nanocups-like morphology. Unlike borocarbonitrides prepared by urea method, gas phase synthesized BC_xN exhibit less surface area and gas adsorption properties.

• Hydrogen is the ultimate clean and green source of energy. Only clean and environment friendly way to produce hydrogen is from water using natural energies such as sunlight. There have been several efforts to produce hydrogen via water splitting using electrolysis of water using solar cell, reforming biomass and photocatalytic and photoelectrochemical water splitting. Photocatalytic water splitting using powder catalyst dispersed in water by simply shining light is one of the most energy effective and easiest ways to obtain H_2 and O_2. We are using spinel based photocatalysts containing "Mn_4O_4 cubane" like structure similar to that found in chlorophyll for oxidation water. Semiconductor based photocatalysts like N doped and N, F co-doped TiO_2, solid solutions of InN-GaN- ZnO, layered MoS_2 etc are also being tried for H_2 evolution.

• Multiferroic oxides are generally considered to be rare because magnetism and ferroelectricity mutually exclude each other as the microscopic origin of both these properties is different. Magnetism arises due to ordering of unpaired spins whereas ferroelectricity occurs due to charge separation in the respective oxides. Magnetism (Spin-driven) induced ferroelectricity is one of the most effective routes which give rise to strong coupling between magnetism and ferroelectricity. Recent studies on ferrites of the general formula $Al_{1-x}Ga_xFeO_3$ (x= 0, 0.5, 1) shows multiferroic behaviour at low temperatures. All of them crystrallize in the orthorhombic structure with the non-centrosymmetric space group $Pna2_1$. The crystal structure contains considerable amount of disorder among the cations and it is invariant with temperature. This family of ferrites are collinear ferrimagnetic (T_N = 200-250K) and exhibit spontaneous electric polarization in the vicinity of ~100 K (below T_N) as obtained from pyroelectric current measurements. The appearance of polar state has been considered on the basis of non-centrosymmetric magnetic ordering arising from the inherent magnetic frustration and it was also evidenced from the studies of temperature dependent Raman spectroscopy. Application of magnetic field shows a considerable effect on the polarization data and hence magnetoelectric effect. Therefore magnetically induced ferroelectric material can give rise to a new direction to design future room temperature multiferroic material which would find many new applications.

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DST UNIT ON NANOSCIENCE

Nanoscience, being an interdisciplinary topic, calls for a multi-faceted approach. The members of the Unit with varied expertise have formed a Group to pursue research activities on different aspects of Nanoscience. In order to boost research interest in nanoscience, many academic activities such as courses in nanoscience, discussion meetings and symposia are being conducted.

The main activities of the Unit are as follows:
Developing new strategies for the synthesis and purification of nanowires and nanotubes; multiwalled and single walled carbon nanotubes, junction nanotubes, nanowires and nanotubes of transition metal oxides, nitrides, carbides and chalcogenides, new precursor routes to metal and semiconductor elemental nanowires, aligned nanotubes.

Graphene, graphene derivatives and graphene analogues of inorganic layered material; synthesis, and properties, graphene based SETs and photo detectors.

Synthesis of metal and semiconductor nanocrystals in colloidal sols as well as at liquid-liquid interfaces, ligand shell modification, core-shell nanocrystals, magic nuclearity nanocrystals, mesoscalar assemblies.

Patterned nanomaterials, Electron beam and AFM-based high-resolution nanolithography.

Thin films of novel functional oxides, transition metal oxides of interest in high Tc superconductivity, synthesis using RF magnetron sputtering, characterization and processing.

Characterization of nano objects using electron and scanning probe microscopy techniques, UV-Vis spectroscopy, X-ray photoelectron spectroscopy.

Characterization of nanomaterials using high-resolution powder X-ray diffraction, RDF from Rietveld analysis, Reflectivity studies on films.

Electrical and magnetic properties of the oxide films as well as on nanocrystalline metal and semiconductor films.

Direct measurement of electrical properties of nanowires and nanotubes coupled to nanoelectrodes drawn using e-beam lithography, Nanocrystals anchored to conducting organic molecules, Surface-enhanced Raman spectroscopy (SERS) by tagging gold and silver nanoparticles to protiens, polypeptides, etc., Diagnostic tools for biology.

Theoretical calculations of conductance, capacitance and current as a function of the external bias, temperature and magnetic field, Effect of the dimensionality and the geometry of the contacts, modelling advanced materials showing rectification and those of interest in spintronics.

ACADEMIC ACTIVITIES

ACADEMIC PROGRAMMES

STUDENT LIFE

EXTENSION PROGRAMMES

LECTURES AND MEETINGS

RESEARCH & DEVELOPMENT

COUNCIL OF MANAGEMENT, ACADEMIC ADVISORY COMMITTEE, PRESIDENTS, HONORARY FELLOWS

ADMINISTRATION

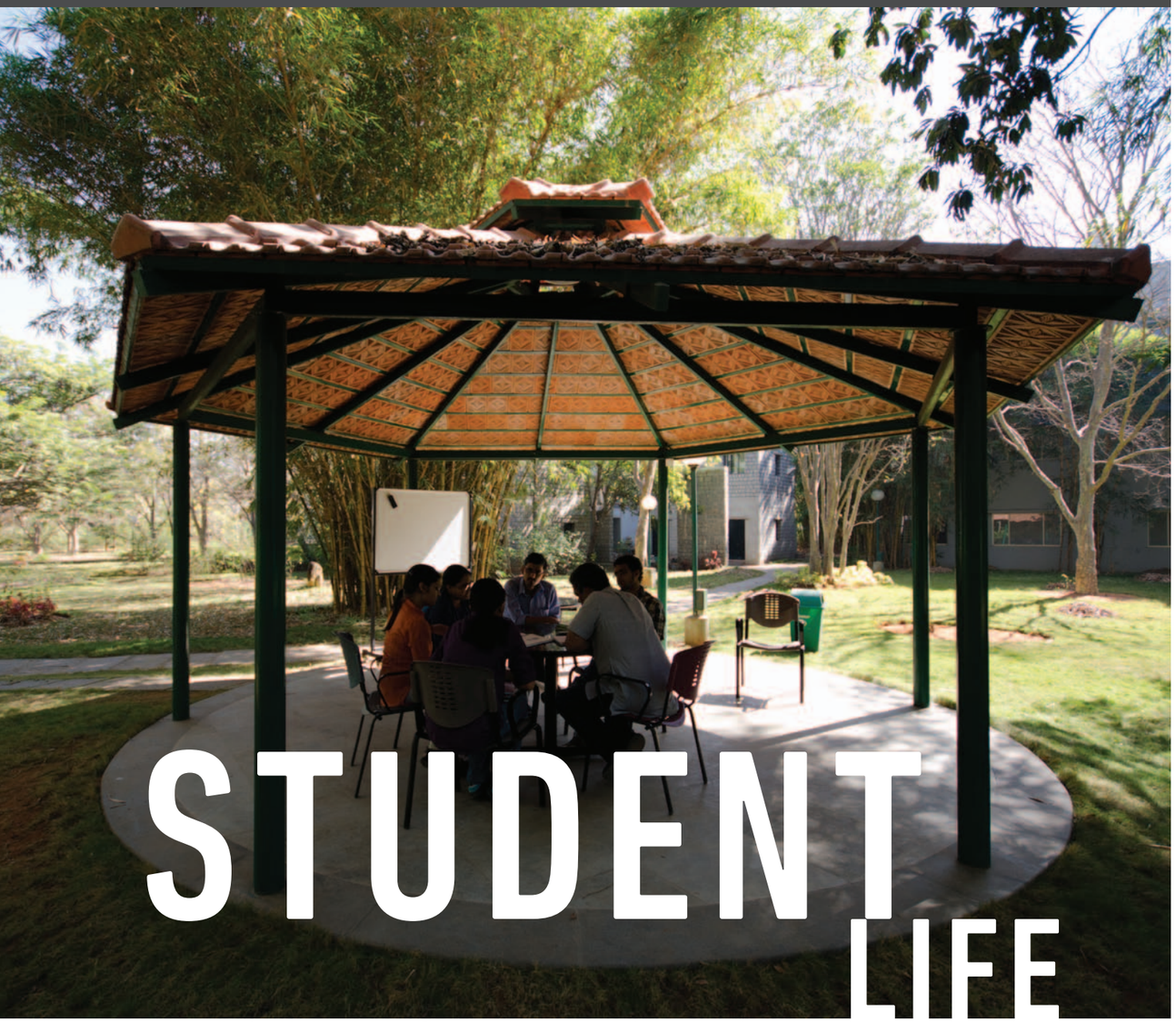
ACADEMIC PROGRAMMES

The Jawaharlal Nehru Centre for Advanced Scientific Research is a globally recognized research institution, and a community comprising of faculty and students working in multidisciplinary areas and diversified units. A body of thinkers and doers, the Centre provides a stimulating and rewarding environment for its students, while allowing unfettered access and interaction with the academic fraternity.

Students willing to attend JNCASR's Integrated PhD, PhD and MS programmes undergo written tests and interviews. Often, young students who participate in the summer programmes have an option to join our degree programmes. The JNCASR approach is to encourage rigorous course work in science and engineering, while stimulating critical thinking, writing, and presentation skills. Established in 1989, the Centre has created a niche for itself in the global scientific community, by achieving commendable progress in just twenty-five years. JNCASR publishes an average of 250-300 publications every year. Its students have presented their work nationally and internationally to great acclaim.

The Centre's alumni of 122 PhDs, and 77 MSs have gone on to do extremely well at IITs, IISERs, Honeywell, and GE, as well as overseas, at NASA, Johns Hopkins, Max Planck, and Cornell.

JNCASR is best suited to talented, strongly motivated students who flourish in a dynamic, intellectually challenging environment. For further information, and admission guidelines, take a closer look at the Centre's website: www.jncasr.ac.in/admit



STUDENT LIFE

> BESIDES RESEARCH IN THE LAB, WHAT I MOST LIKE ABOUT JNC IS THE ENVIRONMENT IT PROVIDES. THE CAMPUS IS LOVELY WITH BAMBOO PATCHES, TREES IN FULL BLOOM AND SMALL FLOWERING PLANTS PROVIDING HABITAT FOR A WIDE VARIETY OF BIRDS AND INSECTS.
> – Sarada Seetharaman, TSU

The JNCASR Student's Residence reflects the vibrant scientific spirit of the Centre. Modern in design, luxurious in amenities, and infused with an atmosphere of vitality and good cheer, it is the perfect environment for the growing scientific mind to relax, and feel entirely at home.

Comfortable rooms set amidst a lush, green campus create a calm and peaceful environment, while a range of student activities and engagements provide stimulation and interaction, for the mind as well as the body. The JNCASR student community takes the collaborative spirit of the Centre to a whole new level – sharing influences, discussing schools of thought, and stimulating new ways of thinking and expression.

Here you will find students from different parts of the country and the world, with, different academic, professional, and cultural backgrounds. Unlike many other research institutes, the relatively small numbers enable meaningful personal relationships, and the informal nature of faculty-student interactions open up a wealth of discussions. Candid discussions over coffee on a broad range of topics provide a greatly enhanced perspective of the world, as do a wealth of like-minded gatherings like book and movie clubs.

Beyond feeding the curious young minds of the Centre, the hostel also provides for their bodies. Far from the conventional picture of undernourished scientific geniuses cooped up in a room, slaving over their theses, a student at JNCASR can choose from a host of sports such as badminton, table tennis, basketball, and football, or sit down to a game of chess, carom, or Scrabble. For the literarily inclined, there is a well-stocked library run by an active Book Club, as well as a literary magazine, Fingerprints, to express students' prose and poetic creations. Dhwani is a popular forum where students screen documentary films and debate subjects ranging from the mundane to the controversial, from the historical to those of current relevance. The Movie Club showcases movies, both popular, as well as classics, every Friday night in an open-air theatre.

The sense of logic and collaboration also extends to the choice of meals at the hostel, as a revolving committee of students directs the menu of the month.

Nourishing, enriching, and engaging, the JNCASR hostel is a mini-picture of an ideal scientific community – one that enjoys life fully, while remaining constantly engaged with scientific problems ranging from the most fundamental to those of a highly applied nature.

THE STUDENTS' RESIDENCE OR THE HOSTEL, LOCATED INSIDE THE CAMPUS, IS LITERALLY A HOME AWAY FROM HOME. BEING HAPPY AND COMFORTABLE IS IMPORTANT FOR A BEING GOOD RESEARCHER; THIS IS WHAT MOTIVATES THE WARDENS AND HOSTEL STAFF TO MANAGE AND MAINTAIN THE HOSTEL AS ONE OF THE BEST IN THE COUNTRY.
– Vini Gautam, CPMU

THE MOVIE CLUB SCREENS ONE HAND-PICKED MOVIE EVERY FRIDAY NIGHT. IF YOU ARE A FAN OF DOCUMENTARIES, A LOVER OF HEALTHY DEBATES, *DHWANI* IS WHERE YOU SHOULD BE EVERY THURSDAY. THE BOOK-CLUB HOSTS NOT ONLY BOOKS ON INTERNATIONAL LITERATURE, BUT ALSO ON VERNACULAR LITERATURE, TO CATER TO EVERY STUDENT'S NEEDS.
– Chandradhish Ghosh, Ph.D. student, ICMS

"ONE COULD ACCIDENTLY STUMBLE INTO THE LECTURE HALL AND END UP LISTENING TO EITHER A WONDERFUL TALK ON THE FASCINATING PROPERTIES OF NANOMATERIALS OR ON THE WAY CIRCADIAN RHYTHMS GOVERN THE BEHAVIORAL PATTERN OF VARIOUS ORGANISMS. VERY FEW INSTITUTIONS OFFER THIS BIRD'S EYE VIEW OF PROGRESS ACROSS ADVANCED DISCIPLINES OF SCIENCE."
– Bharat, MBGU

"THE STRIKING FEATURE OF JNC IS THE HIGHLY INFORMAL NATURE OF THE FACULTY-STUDENT INTERACTION. IN CONTRAST TO MANY UNIVERSITIES ABROAD, MOST STUDENTS IN JNC GET TO INTERACT WITH THEIR ADVISORS ON A DAILY BASIS. THE MANY DISCUSSIONS I HAVE HAD WITH MY ADVISOR AND RESEARCH GROUP OVER COFFEE ON A BROAD RANGE OF TOPICS HAVE GREATLY ENHANCED MY VIEW OF THE WORLD."
– Saikishan Suryanarayanan, Ph.D. student, EMU

EXTENSION PROGRAMMES

In addition to pursuing research in various contemporary areas, JNCASR also conducts several Science Outreach and Fellowship Programmes. One such flagship activity is the Summer Research Fellowship Programme for young students. Since its inception in 1990, around 1,700 students have benefitted from this programme. Every year, 120-130 fellowships are offered. It enables students to be inspired by research at a very early stage of their education. With the aim to make this programme globally visible, JNCASR has collaborated with the Third World Academy of Sciences, Regional Office for Central and South Asia, to make the programme accessible to undergraduate students in developing countries in South Asia and Africa which will expose young students in the region to the research culture in advanced areas of science and engineering.

There is an urgent need to sharpen the research skill of students from an undergraduate level, and the Centre, in its own way, attempts to provide regular Chemistry and Biology research training at the Centre. The Project Oriented Chemical Education (POCE) and the Project Oriented Biological Education Programme (POBE) have completed 9 and 7 years respectively. Ten meritorious students are selected from across the country for each of these programmes every year. As part of this, students undertake small project in association with faculty members of the Centre during their mid-semester breaks. They also attend special lectures and seminars at the Centre. On the successful completion of their training, they are awarded a Diploma certificate in Chemistry or Biology. Many of them have joined reputed institutions in India and abroad for pursuing scientific career.

The Centre also offers Visiting Fellowships to teachers and research scientists from various educational institutions and R&D laboratories to work with the faculty and honorary faculty of JNCASR. The aim is to facilitate exposure to learning techniques not available in their own institutions and also encourage future collaborations with the Centre's faculty. Every year 10-15 fellowships are offered under this programme. This programme has been welcomed by many researchers in the country as they are able to develop their skills at their parent establishment after undergoing training and research at JNCASR. This programme has been immensely beneficial to faculty working in government universities or educational institutions in our country since most of these universities or institutions do not have state-of-the-art facilities like JNCASR.

Apart from the above felowship programmes, the Centre and its faculty have been actively popularizing science for the students between the age 13-18 years. Every year JNCASR organizes National Science Day by arranging seminars, workshops, visits to laboratories; exposing, both, teachers and students to current research in various fields of science.

LECTURES AND MEETINGS

MEMORIAL LECTURES

A V RAMA RAO FOUNDATION LECTURES IN CHEMISTRY

Phosphorus-Supported Ligands: Versatile Coordination Platforms for the Assembly of Molecular Materials, Prof. V. Chandrasekhar, Department of Chemistry, Indian Institute of Technology Kanpur; May 13, 2011;

PRIZE LECTURE

Hybrid Nanomaterials for Sensing and Light Energy Conversion, Prof. George Thomas, School of Chemistry, Indian Institute of Science Education and Research, Trivandrum, May 13, 2011.

Fluorescent Molecular Architectures with Exceptional Properties, Dr A Ajay Ghosh, CSIR-Outstanding Scientist, Chemical Sciences & Technology Division, NIIST, Trivandrum; May 16, 2012.

PRIZE LECTURE

Luminescent Nano Materials for Photonic Applications, Dr Amitava Patra, Department of Materials Science, Indian Association for the Cultivation of Science, Kolkata, May 16, 2012.

PROF V RAMALINGASWAMI MEMORIAL LECTURE

The Inside Story of the Impoverished Gut, Dr Gopinath Balakrish Nair, Director, NICED, Kolkata, July 8, 2011.

PROF CNR RAO ORATION AWARD LECTURE 2011

Modifying materials for super-efficient Solar Cells and Light Emitting Diodes, Prof S M Shivaprasad, Chemistry and Physics of Materials Unit, JNCASR, August 5, 2011.

ISAAC NEWTON LECTURE

From Volta to Lithium and Beyond, Prof Jean Marie Tarascon, Professor of Chemistry, Université de Picardie Jules Verne, Amiens, France, August 22, 2011.

DAE RAJA RAMANNA LECTURES IN PHYSICS 2011

Solving Quantum Field Theory using Black Holes in one higher dimension, Prof Spenta R Wadia, Director, International Centre for Theoretical Sciences, TIFR, Mumbai; May 16, 2012;

PRIZE LECTURE

Condensed Matter Physics with Cold Atoms: From Bose Condensation to Synthetic Non-Abelian Gauge Fields, Prof. Vijay B Shenoy, Associate Professor, Centre for Condensed Matter Theory, Department of Physics, IISc, Bangalore, May 16, 2012.

ISRO- SATISH DHAWAN LECTURE 2011

Lords of 33 villages: Mysore under the wodeyars", Mr. Vikram Sampath, October 14, 2011.

ICMS SHEIK SAQR MATERIALS LECTURE

Dilute Ferromagnetic Oxides and d-zero Magnetism; what can we believe?, Prof. J. M. D. Coey, School of Physics and CRANN, Trinity College, Dublin 2, Ireland, October 20, 2011.

PROF M K CHANDRASHEKARAN MEMORIAL LECTURE

A Brief History of Internal Time, Prof Serge Daan, Niko Tinbergen distinguished honorary chair in Behavioral Biology, Linnaeusborg, University of Groningen, The Netherlands, January 19 - 20, 2012.

ANNUAL CHEMISTRY LECTURE

Chemistry Inspired by Interstellar Molecules, Prof Herbert W Roesky, University of Gattingen, Institute of Inorganic Chemistry, February 23, 2012.

ICMS-SECOND ANNUAL MATERIALS SCIENCE LECTURE

Prof Satishchandra B Ogale, Centre of Excellence in Solar Energy, Physical and Materials Chemistry Division, National Chemical Laboratory (CSIR-NCL), Pune, March 20, 2012.

SPECIAL LECTURES

Lattice kinetic theory across scales: from fluid turbulence to electron flows in grapheme, Prof. Sauro Succi, Research Director, IAC-CNR, Rome, Italy, October 24, 2011.

Conference on Science Communication Addressing Women's Issues, Mr A P Deshpande, NCSC, Mumbai, January 7 - 8, 2012

Women, Law and Society, Justice Mrs Sudha V Manohar, Former Judge of Supreme Court of India, JNCASR, March 26, 2012

Can the Poor afford Solar Lamps, Dr Harish Hande, January 10, 2012

Recent Trends in Neurosurgery, Dr D V Rajakumar, Fortis Hospital, Bangalore, April 11, 2012.

IPR LECTURE

IP Valuation, Ms. Anjana Vivek, Founder, VentureBean Consulting, November 9, 2011.

ANNUAL FACULTY MEETING LECTURES

Phenomenological theory of high-temperature superconductivity in the cuprates, Prof. Chandan Dasgupta

Genetics of an epilepsy precipitated by tactile and temperature cues, Prof. Anuranjan Anand

Self-Assembly approach towards Functional Organic Materials, Dr. Subi Jacob George

The Curious Case of NiS: Is it a metal or is it not!, Prof. D D Sarma

Disorder, Freezing and Spiral Dynamics in the complex Ginzburg – Landau Equation, Dr. Subir K Das

MEETINGS

- *2nd National Molecular Virology Meeting,* Prof C Durga Rao, IISc, April 29-30, 2011.
- *Science Outreach Programme – Summer 2011,* Prof. K.S. Valdiya, JNCASR, May 18-19, 2011.
- *Entertainment and Universality in Jets and Plumes: an Integral Approach,* Dr. Sourabh Diwan, Participants: Narasimha Roddam, S.M. Deshpande on May 26, 2011.
- *Indo-US Workshop on "New Functional Materials",* Manali, June 2-6, 2011.
- *Indo-US-Symposium on "New Functional materials Synthesis, Properties and methods",* Prof Ashok K Ganguli, IIT-D, June 2-7, 2011.
- *Afro-Asia Workshop on "Advanced Topics in Chemistry",* June 13-17, 2011.
- *EICOON Meeting,* June 13-17, 2011.
- *National Conference on "Nanoscience and Engineering for Better Ceramics NanoSEC-2011",* Prof Arun M Umarji, IISc, June 23-24, 2011.
- *Third Management Board Meeting,* June 24, 2011.
- *TSU In-House Symposium,* August 4, 2011.
- *Research Conference on Chemistry of Functional Materials,* Prof R Murugavel, IIT-Bombay, August 12-14, 2011.
- *Theoretical and Experimental Immunology,* Prof Dipankar Nandi, IISc, August 16, 2011.
- *7th Kannada Vijnana Sammelana,* Prof K I Vasu, September 15-17, 2011.
- *JNCASR Research Conference,* Kochi, October 1-3, 2011.
- *JSPS/DST Workshop in Graphene,* Japan October 13-15, 2011.
- *Meeting on Chemistry & Physics of Advanced Materials,* Prof AJ Paul, IACS, Kolkata, October 29-31, 2011.
- *Indo-Australia Joint Symposium on Nanomaterials,* at RMIT, Melbourne Australia, November 2-4, 2011.
- *Meeting with Dr Caroline Ash,* Sr Editor, Science Magazine, AAAS, November 4, 2011.
- *National Conference, PLD-2011,* Prof S B Krupannidhi, IISc, November 9 - 11, 2011.
- *5th ASIAHORCs Meeting,* JNCASR, November 27, 2011.
- *International Conference on "Dynamics of Phase Transformation",* November 28-30, 2011.
- *Workshop on magnetism: practice and theory,* Dr Dipankar Das Sarma, IISc, November 30 - December 4, 2011.
- *Winter School on Physics and Chemistry of Materials,* convenors: Dr. A. Sundaresan and Prof. Swapan K. Pati, December 5-9, 2011,JNCASR
- *ICMS Winter School,* JNCASR, December 5 - 10, 2011.
- *8th Indo-Australia Biotechnology Conference on Stem Cell Biology,* December 7 - 9, 2011.
- *Opening scientific doors: exploration of potential areas for collaboration in chemistry and physics,* Discussion Meeting with George Town University, USA, January 5 – 7, 2012.
- *Indo-UK Excitonic Solar Cell Meeting,* Prof K S Narayan, January 9 – 11, 2012.
- *Indo-US Workshop and Seminar on Malaria,* January 16-18, 2012.
- *EOBU Symposium,* JNCASR, Bangalore, January 19 - 20, 2012.
- *Contemporary Issues in Condensed Matter Science,* Prof Rahul Pandit, January 30 - February 1, 2012.
- *Unifying Concepts in Materials,* James A Krumhansl School and Symposium (JAKS-2012), Prof Srikanth Sastry, JNCASR, Bangalore, January 30 – February 5, 2012.
- *20th Discrete Simulations of Fluid Dynamics (DSFD),* convenor: Dr. Santhosh Ansumali, JNCASR, 2012.
- *6th RNA Group Meeting,* Prof Sanmitra Das, March 30 - 31, 2012.
- *Indian Society of Neuro-Oncology (ISNOCON 2012),* Dr Vani Santhosh, April 6 - 8, 2012.

FLUID DYNAMICS COLLOQUIA

Concentration Dependent Dynamics Of Semi-Dilute DNA Solutions, Dr J Ravi Prakash, Department of Chemical Engineering, Monash University Melbourne, Victoria, Australia, July 8, 2011.

Long-range spatial correlations in sheared colloidal glasses, Dr Vijayakumar K Chikkadi, Institute of Physics, University of Amsterdam, The Netherlands, August 10, 2011.

Modelling bistability of mid-latitude atmospheric jets, Dr Manikandan Mathur, Laboratoire des Ecoulements Geophysiques et Industriels, Grenoble, France, August 19, 2011.

Serrated flow in nanotether formation from vesicles, Dr B Ashok, Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Hyderabad, August 16, 2011.

Multiphase Lattice Boltzmann simulation of buoyancy-driven flow of two immiscible fluids in an inclined channel, Dr. Kirti Chandra Sahu, Department of Chemical Engineering, Indian Institute of Technology Hyderabad, India, October 3, 2011.

Stability of spinning, self-gravitating, rubble-pile asteroids, Prof. Ishan Sharma, Assistant Professor, Department of Mechanical Engineering, IIT, Kanpur, November 11, 2011.

Numerical Simulation of HP Vane cascade under free stream turbulence, Dr Sanjiva Lele and Dr R Bhaskaran, Department of Mechanical Engineering and Astronautics and Aeronautics, Stanford University, November 18, 2011.

The PSE-3D instability analysis methodology for flows depending strongly on two and weakly on the third spatial dimension, Pedro Paredes, Vassilios Theofilis and Daniel Rodra guez, School of Aeronautics, Universidad Politecnica de Madrid, E-28040 Madrid, Spain 2 Division of Engineering and Applied Science, California Institute of Technology, Pasadena CA, USA, November 30, 2011.

On the relation between the equation for large-eddy simulation of turbulent flow and for weakly nonlinear evolution of disturbances for flows in transition, Prof V Vasanta Ram, Ruhr University, Bochum, November 22, 2011.

Climate Science, Waves, and PDEs for the Tropics: Observations, Theory, and Numerics, Prof Andrew J Majda, Morse Professor of Arts and Sciences, Department of Mathematics and Climate, Atmosphere, Ocean Science (CAOS), Courant Institute of Mathematical Sciences, New York University, December 9, 2011.

Some insights into wetting hysteresis - experiments and modeling, Prof Mahesh Panchagnula, Department of Applied Mechanics, IIT Madras, January 13, 2012.

Optimal Path to Turbulence in Shear Flows, Prof Dan Henningson, Professor in Fluid Mechanics, FLOW, KTH Mechanics, Sweden, January 17, 2012.

Drag reduction and the nonlinear dynamics of Newtonian and viscoelastic turbulence, Prof Michael D Graham, Department of Chemical and Biological Engineering University of Wisconsin-Madison, USA, January 24, 2012.

Some insights into wetting hysteresis - experiments and modeling, Prof Mahesh Panchagnula, Department of Applied Mechanics, IIT Madras, January 24, 2012.

Generation of solitary waves in an oceanic thermocline by internal gravity waves, Prof Chantal Staquet, Laboratory of Geophysical and Industrial Fluid Flows (LEGI), Grenoble, France, February 14, 2012.

Dynamical systems approach to the investigation of thermoacoustic instabilities, Dr Priya Subramanian, Department of Aerospace Engineering, Indian Institute of Technology Madras, March 21, 2012.

Non-normal and nonlinear instabilities in thermo-acoustic interactions, Prof Sathesh Mariappan, Department of Aerospace Engineering, Indian Institute of Technology Madras, May 23, 2012.

INTELLECTUAL PROPERTY

RESEARCH & DEVELOPMENT

Journey through various sections of this brochure will give an overview of the vast spectrum of research and development, education and training activities pursued at the Centre. As per the recent survey based on the standard performance-indicators and parameterized by the quality scientific publications, the Centre has been recognized as one of the foremost research institute in the country.

Centre provides a vibrant academic ambience with excellent state-of-the-art research facilities hosting highly intellectual and motivated faculty and research staff. Researchers at the Centre have been honoured with national and international recognitions for their outstanding contribution to the scientific world. The Centre publishes, around 250 scientific papers annually in national and international peer-reviewed journals with reasonably high impact factors.

Centre receives substantial national and international funding to solve cutting edge research problems in addition to generating reasonable income from internal resources to supplement the external funding. It has undertaken many initiatives to translate the excellence achieved in the academic endeavor for addressing problems in various sectors. It promotes interdisciplinary collaborations with various international leading research institutions around the globe and has led to periodic breakthroughs of technological relevance. Centre's inventions and solutions have been explored in the areas ranging from electronics-technology to manufacturing, and in pharmaceutical and health industries for disease-diagnostics and drug development.

In view of providing access to the wide array of scientific and engineering expertise available at the Centre and to encourage the national and multinational business entities, Centre also extends consultancy services in the research areas pursued at the Centre. Some of our faculties are consultants for leading firms.

To explore the possibilities for collaborations, sponsored projects, contract and consultancy services, you are welcome to contact:

Dean
Research & Development
JNCASR, Jakkur, Bangalore 560064

Email: deanrandd@jncasr.ac.in, Telephone: 91-80-22082681

INTELECTUAL PROPERTY

Intellectual property is an integral part of the technological innovations in the knowledge based economy driving socio-economic development. Technological innovations are crucial for maintaining successful technological leadership. Recognizing the value of application oriented research and intellectual property (novel ideas and inventions in the form of processes, products, designs, software, multimedia packages, etc.) development and to foster its access to industry, the Centre has constituted an IP Management Committee to address issues pertaining to generation, valuation, protection and valorization of IP. It has framed an enabling mechanism for managing IP that blend with its mission.

The dynamic multidisciplinary, sustained and extensive collaborative R&D at the Centre has resulted in 41 inventions/technologies in the areas of Nanotechnology, Biotechnology, Electronics and Aeronautics. The scope of collaboration in developing these inventions spreads across laboratories and departments within the Centre and extended to academia and industry within India and abroad. This reflects the extensive collaborative environment created at the Centre.

The Centre has filed 114 national and international patent applications and obtained 20 patents and the rest are at various stages of prosecution. Centre was successful in licensing 13 inventions to the industry to transform nascent scientific discoveries into products and services for the benefit of public good and efforts are on for commercializing the rest of the inventions. This illustrates that, the Centre not only filed and secured a very high per capita number of patents, but has also licensed a high percentage of them to industry.

The inventions/technologies disclosed to the public through patent publications are listed below to reflect the diversity and to explore the possibilities of: (a) licensing inventions, (b) inviting collaborations, and (c) for extending consultancy services.

Invention: **Photo Responsive Organic Field Effect Transistor**
Inventor: Kavasssery Narayan Sureswaran
Patents granted to date: **USA (No. 6992322)**

Invention: **Use Of Hydroxydiphenyl Ether Class Of Chemicals, As Exemplified By Triclosan, As An Antimalarial And Identification Of Fatty Acid Synthesis At Its Target**
Inventors: Namita Surolia, Avadesh Surolia
Patents granted to date: **South Africa (No. 2001/2305), Australia (No.780085), Europe (No. 1137386)**

Invention: **Modulators (Inhibitors/Activators) Of Histone Acetyltransferases**
Inventors: Tapas K Kundu, Alamelu Vaidhyanathan, Karanam Balasubramanyam, Venkatesh Swaminathan
Patents granted to date: **India (No. 212171), USA (Nos. 7332629, 7750047)**

Invention: **Process For Extraction Of Superior Quality Plasmid DNA**
Inventor: Ranga Udaykumar
Patents granted to date: **India (No. 193223)**

Invention: **A Novel Composition To Be Used In The Field Of Molecular Biology**
Inventor: Ranga Udaykumar
Patents granted to date: **India (No. 221411)**

Invention: **Polyisoprenyl Benzophenones As Inhibitors Of Histone Acetyl Transferases And Uses Thereof**
Inventors: Tapas Kumar Kundu, Balasubramanyam Karanam, Mantelingu Kempegowda, Mohammad Altaf, Swaminathan Venkatesh, Radhika Ashish Varier
Patents granted to date: **India (No. 223720), USA (No. 7402706), EPO (No. 1694622)**

Invention: **Highly Specific Polyclonal Antibodies Of Individual Core Histone And Uses Thereof**
Inventors: Tapas Kumar Kundu,Chandrima Das, Radhika Ashish Varier, Febitha Kandan Kulangara
Patents granted to date: **India (No. 239873)**

Invention: **Derivatives Of 4, 6-Disubstituted 1, 2, 4-Triazolo-1, 3, 4-Thiadiazole, A Process And Uses Thereof**
Inventors: Tapas Kumar Kundu, Radhika Ashish Varier, Kanchugarakoppal Subbegowda Rangappa, Badi Sri Sailaja, Nanjundaswamy shivananju, Basappa
Patents granted to date: **India (No. 245033), EPO (No. 1945648)**

Invention: **Site-Specific Inhibitors Of Histone Methyltransferase (HMtase) And Process Of Preparation Thereof**
Inventors: Tapas Kumar Kundu, Selvi Ruthrotha Bharatha Vikru, Hari Kishore Annavarapu, Mantelingu Kempegowda
Patents granted to date: **USA (Nos. 7875741, 8003698)**

Invention: **A High Sensitivity Assay For Molecular Typing Of Biological Sample, Probes And A Kit Thereof**
Inventors: Ranga Udaykumar, Chandrabhas Narayana, Jayasuryan Narayana
Patents granted to date: **South Africa (No. 2009/03128), USA (No. 8,227,590)**

Invention: **A Mirror Adapted In Microscope To Perform Surface Enhanced Raman Spectroscopy, A Microscope And Methods Thereof**
Inventors: Chandrabhas Narayana, Pavan Kumar Gopalapura Venkataramu
Patents granted to date: **USA (No. 8,179,525 B2)**

Invention: **Methods And Compositions For The Separation Of Single-Walled Carbon Nanotubes**
Inventors: Chintamani Nagesa Ramachandra Rao, Subi Jacob George, K Venkata Rao, Rakesh Voggu.
Patents granted to date: **USA (No. 8246928)**

Invention: **Intrinsically Fluorescent Carbon Nanospheres And A Process Thereof**
Inventors: Tapas Kumar Kundu, Eswaramoorthy Muthusamy, Selvi Bharatha Ruthrotha Vikru, Dinesh Jagadeesan

Invention: **Nanoparticles Composition And A Process Thereof**
Inventor: Chandrabhas Narayana

Invention: **A Template Free Metal, Polymer Free Metal Nanosponge And A Process Thereof**
Inventors: Eswaramoorthy Muthusamy, Saikrishna Katla

Invention: **Tat DNA Sequences, Gene Constructs, Vaccine And Processes Thereof**
Inventor: Ranga Udaykumar

Invention: **SERS Active Paper Substrate, A Process And A Method Thereof**
Inventors: Kulkarni Giridhar Udapi Rao, Anurag Gupta, Balasubramanian Karthick

Invention: **Polynucleotide Sequences And Processes Thereof**
Inventors: Kaustuv Sanyal, Sreedevi Padmanabhan, Jitendra Thakur

Invention: **Optimal Wing Planforms For Reducing The Induced Or Total Drag Of The Wing Of An Aircraft Driven By Wing-Mounted Tractor Propellers/Rotors**
Inventors: Roddam Narasimha, Madhusudan Deshpande, Praveen Chandrashekarappa, Rakshith Belur Raghavan

Invention: **Inhibition Of Histone Acetyltransferases By CTK7A And Methods Thereof**
Inventors: Tapas Kumar Kundu, Mohammed Arif, Kempegowda Mantelingu, Gopinath Kodaganur Srinivasachar

Invention: **A Synthetic Cyclic Peptide And A Process Thereof**
Inventor: Govindaraju Thimmaiah

Invention: **Highly Specific Antibodies, Composition And Methods Thereof**
Inventors: Tapas Kumar Kundu, Jayasha Shandilya, Parijat Senapati

Invention: **Artificial Retina Device**
Inventors: Kavasssery Narayan Sureswaran, Vini Gautam, Monojit Bag

Invention: **Vector, Vector Combinations, Methods And Kit Thereof**
Inventor: Ranga Udaykumar

Invention: **Formation Of Palladium Sulfide**
Inventors: Kulkarni Giridhar Udapi Rao, Boya Radha

Invention: **Palladium Thiolate Bonding Of Carbon Nanotubes**
Inventors: Kulkarni Giridhar Udapi Rao, Timothy S Fisher, Stephen L Hodson, Thiruvelu Bhuvana

Invention: **Method For The Diagnosis Of Higher And Lower Grade Astrocytoma Using Biomarkers And Diagnostic Kit Thereof**
Inventors: Kumaravel Somasundaram, Paturu Kondaiah, Vani Santosh, Sridevi Hegde, Alangar Sathyaranjandas Hegde, Manchanahalli Rangaswamy Satyanarayana Rao

Invention: **Self Assembly Of Naphthalene Diimide Derivatives And Process Thereof**
Inventors: Govindaraju Thimmaiah, Manjula Basavanna Avinash, Makam Pandeeswar

Invention: **Bulk Heterojunction/Electrolyte Polymers As Novel Biocompatible Photoactive Multi Color-Sensing Technology**
Inventors: Kavasssery Sureswaran Narayan, Vini Gautam, Monijit Bag

Invention: **Manufacturing Strain Sensitive Sensors And/Or Strain Resistant Conduits From A Metal And Carbon Matrix**
Inventors: Kulkarni Giridhar Udapi Rao, Boya Radha, Abhay A Sagade

Invention: **Spectroscopic Probing Of The Dynamic Self-Assembly Of An Amphiphilic Naphthalene Diimide Exhibiting Reversible Vapochromism**
Inventors: Subi Jacob George, Mohit Kumar

Invention: **Hydrogen Sorbent Materials**
Inventors: Subi Jacob George, Kotagiri Venkata Rao

Invention: **Chromophores For Detection Of Volatile Organic Compounds**
Inventors: Subi Jacob George, Mohit Kumar

Invention: **Development Of Lipophilic Cationic Glycopeptide Antibiotics And Their Enhanced Activity Against Gram Positive And Gram Negative Bacteria**
Inventors: Jayanta Haldar, Yarlagadda Venkateswarlu, Akkapeddi Padma

Invention: **A Device For Hydrogen Sensing And A Method Thereof**
Inventors: Giridhar U Kulkarni, Ritu Gupta, Abhay A Sagade

Invention: **A Novel Process For Micropattern Generation On Polymer Thin Films Using Pulsed Laser Diffraction**
Inventors: Giridhar U Kulkarni, Ashutosh Sharma, Ankur Verma

In addition to above, Indian Provisional Patent Applications have been filed for the inventions/ technologies of:
- Kavasssery Sureswaran Narayan, Anshuman Jyothi Das
- Giridhar U Kulkarni, Narendra Kurra, Abhay A Sagade
- Ranga Udaykumar, Asokan Mangaiarkarasi
- Subi Jacob George, Kotagiri Venkata Rao
- Tapas Kumar Kundu, Anne-Laurence Boutillier, Snehajyoti Chatterjee, Muthusamy Eswarmoorthy, Puspak Mizar, Chantal Mathis, Jean-Christophe Cassel, Romain Neidl, Mohankrishna Dalvoy Vasudevarao, Vedamurthy Bhusainahalli Maheswarappa

Some of the inventions/technologies licensed on non-exclusive/exclusive basis are as follows:
- Modulators (Inhibitors/Activators) of Histone Acetyltransferases
- Artificial Retina Device
- Bulk Heterojunction/Electrolyte Polymers as Novel Biocompatible Photoactive Multi Color-Sensing Technology
- Methods and Compositions for the Separation of Single-Walled Carbon Nanotubes
- Formation of Palladium Sulfide
- Manufacturing Strain Sensitive Sensors and/or Strain Resistant Conduits from a Metal and Carbon Matrix.
- A Novel Process For Micropattern Generation On Polymer Thin Films Using Pulsed Laser Diffraction.
- Chromophores For Detection Of Volatile Organic Compounds
- Hydrogen Sorbent Materials
- A Novel Process for Micropattern Generation on Polymer Thin Films Using Pulsed Laser Diffraction
- Direct Laser Ablative Patterning Of Graphite To Produce Graphene Ribbons
- Novel Biocompatible Julolidine Conjugates For Selective Copper Detection Using Near Infrared And Fluorescence Detection
- A High Sensitivity Assay for Molecular Typing of Biological Sample, Probes and a Kit Thereof

The Centre also holds Copyright over a number of educational monographs and multimedia packages on interesting areas in science and technology besides registering one Industrial Design for 'Wings for Propeller Driven Aircraft' designed by Roddam Narasimha, Madhusudan Deshpande, Praveen Chandrashekarappa and Rakshith Belur Raghavan.

IPR activities constitute a steadily growing important component of our Centre, especially in the international scenario. Centre's IP has strengthened the institution's reputation, credibility, public image in addition to generating a reasonable amount of revenue to the Centre and inventors. The continued commitment of our researchers and their collaborators in focusing on development of future inventions/technologies towards driving the economic engines of innovation and addressing global challenges is highly appreciable.

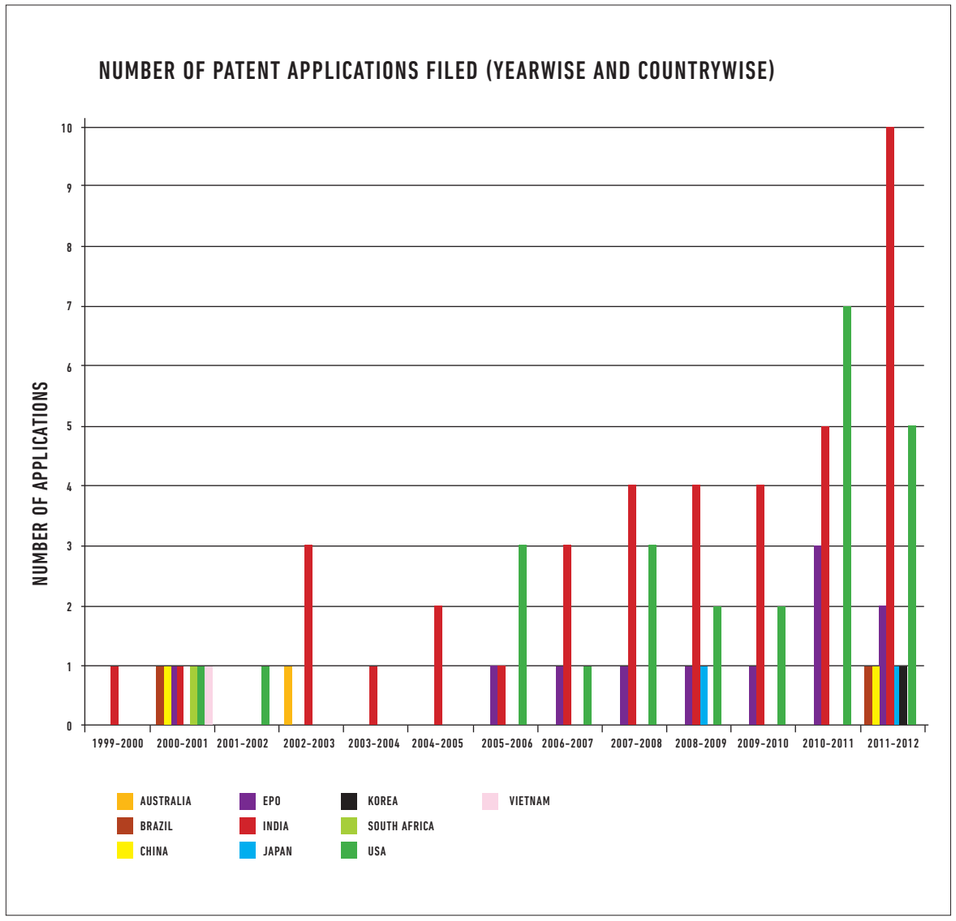


Fig. 1 : Tat inhibition enhances RFP expression. Red fluorescent protein expression is suppressed in HEK293 cells in the presence of Tat. DRB, a small molecule inhibitor of CDK9, a cellular factor critical for Tat function, can reverse the Tat-mediated suppression of RFP

International Patent Application No. PCT/IB2011/053081

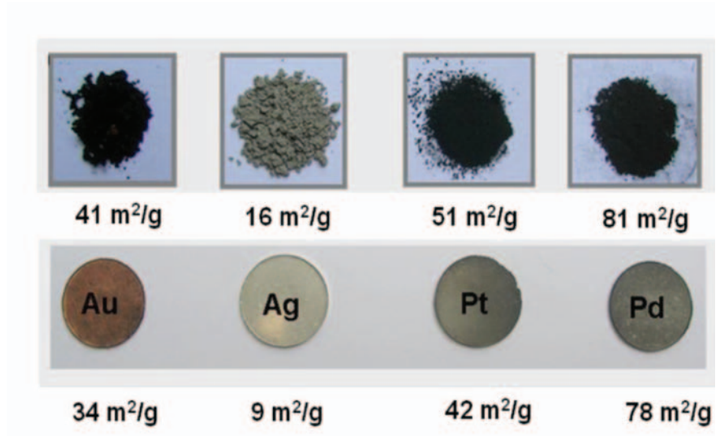


Fig. 2: Photographs of the sponges and sponge pellets with their respective surface areas. (Pellets are made by applying a pressure of 10kN).

International Patent Application No. PCT/IN2009/000266

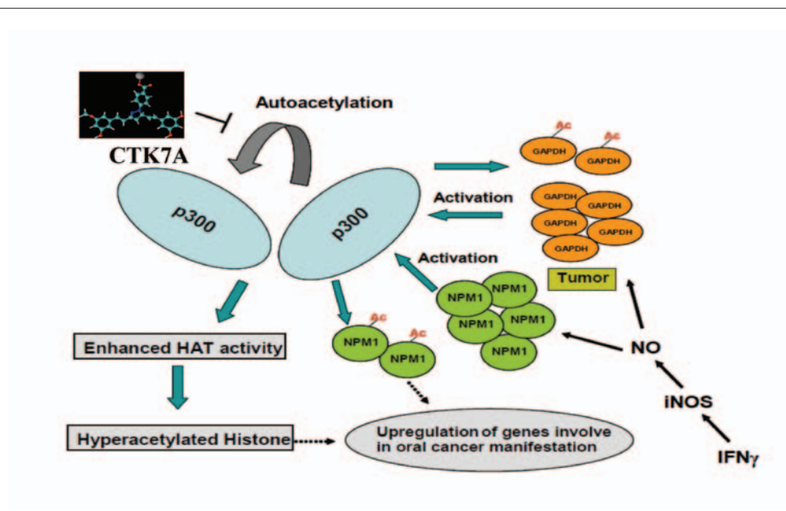


Fig. 3 : IFNγ mediated nitric oxide production enhances the expression of NPM1 and GAPDH which further activate the histone acetyltransferase p300 by inducing the autoacetylation. Highly active p300 hyperacetylates histones as well as NPM1 that cause the expression of genes required for oral cancer manifestation. Inhibition of p300 mediated autoacetylation by a water soluble inhibitor, CTK7A reduces the oral tumor growth in xenografted mice model.

International Patent Application No. PCT/IB2010/053998

PUBLICATIONS

CHEMISTRY OF PHYSICS AND MATERIALS UNIT

Bhuvana, T; Kumar, A; Sood, A; Gerzeski, RH; Hu, J; Bhadram, VS; Narayana, C.; Fisher, T. S.; Contiguous Petal-like Carbon Nanosheet Outgrowths from Graphite Fibers by Plasma CVD. **ACS Applied Materials & Interfaces, 2,** 644, 2010.

Nag, A; Raidongia, K; Hembram, KPSS; Datta, R; Waghmare, UV; Rao, CNR; Graphene Analogues of BN: Novel Synthesis and Properties. **ACS Nano, 4,** 1539, 2010.

Krishna, KS; Sandeep, CS Suchand; Philip, R; Eswaramoorthy, M; Mixing Does the Magic: A Rapid Synthesis of High Surface Area Noble Metal Nanosponges Showing Broadband Nonlinear Optical Response. **ACS NANO, 4,** 2681, 2010.

Chaturbedy, P; Jagadeesan, D; Eswaramoorthy, M; pH-Sensitive Breathing of Clay within the Polyelectrolyte Matrix. **ACS NANO, 4,** 5921, 2010.

Radha, B; Kulkarni, GU; Patterned Synthesis of Pd4S: Chemically Robust Electrodes and Conducting Etch Masks. **Advanced Functional Materials, 20,** 879, 2010.

HSSR, Matte; A, Gomathi; AK, Manna; DJ, Late; R, Datta; SK, Pati; and CNR, Rao; Graphene analogues of MoS_2 and WS_2, **Angewandte Chemie International Edition 49,** 4059 (2010).

Palnitkar, UA; Kashid, RV; More, MA; Joag, DS; Panchakarla, LS; Rao, CNR; Remarkably low turn-on field emission in undoped, nitrogen-doped, and boron-doped graphene. **Applied Physics Letters, 97,** 063102, 2010.

Kumar, P; Kumar, M; Shivaprasad, SM; (7x7) reconstruction as barrier for Schottky-barrier formation at the Ga/Si(111) interface. **Applied Physics Letters, 97,** 122105, 2010.

Rao, KV; Jayaramulu, K; Maji TK; George, SJ; Supramolecular hydrogels and high aspect-ratio nanofibers through charge-transfer induced alternate co-assembly of a new aromatic donor-acceptor pair in water. **Angewandte Chemie International Edition, 49,** 4218, 2010.

Arun, N; Mukhopadhyay, S; Narayan, KS; Monitoring intermediate states of bacteriorhodopsin monolayers using near-field optical microscopy. **Applied Optics, 49,** 1131, 2010.

Kumar, P; Jithesh, K; Shivaprasad, SM; Ga induced superstructures as templates for lattice matched hetroepitaxial growth of GaN on Si(111) substrate. **Applied Physics Letters, 97,** 221913, 2010.

Raidongia, K; Nag, A; Sundaresan, A; Rao, CNR; Multiferroic and magnetoelectric properties of core-shell $CoFe_2O_4$@$BaTiO_3$ nanocomposites. **Applied Physics Letters, 97,** 062904, 2010.

Nie, Y; Wang, Y; Pan, JS; Mehta, BR; Khanuja, M; Shivaprasad, SM; Sun, CQ; CuPd interface charge and energy quantum entrapment: A tight-binding and XPS investigation. **Applied Surface Science, 257,** 727, 2010.

Mallik, AK; Binu, SR; Satapathy, LN; Narayana, C; Seikh, Md M; Shivashankar, SA; Biswas, SK; Effect of substrate roughness on growth of diamond by hot filament CVD. **Bulletin of Materials Science, 33,** 251, 2010.

Krishna, KS; Vivekanandan, G; Ravinder, D; Eswaramoorthy, M; ZnO: a versatile template to obtain unusual morphologies of silica, gold and carbon nanostructures. Chemical Communications, 46, 2989, 2010.

Datta, KKR; Kulkarni, C; Eswaramoorthy, M; Aminoclay: a permselective matrix to stabilize copper nanoparticles. **Chemical Communications, 46,** 616, 2010.

Jayaramulu, K; Kanoo, P; George, SJ; Maji, TK; Tunable emission from a porous metal-organic framework by employing an excited-state intramolecular proton transfer responsive ligand. **Chemical Communications, 46,** 7906, 2010.

Sanghamitra, NJM; Varghese, N; Rao, CNR; Effect of curcumin and Cu^{2+}/Zn^{2+} ions on the fibrillar aggregates formed by the amyloid peptide and other peptides at the organic-aqueous interface. **Chemical Physics Letters, 496,** 104, 2010.

Bhattacharya, S; Shivaprasad, SM; Gajbhiye, NS; Variation of magnetic ordering in ε-Fe_3N nanoparticles. **Chemical Physics Letters, 496,** 122, 2010.

Choudhury, D; Das, B; Sarma, DD; Rao, CNR; XPS evidence for molecular charge-transfer doping of graphene. **Chemical Physics Letters, 497,** 66, 2010.

Subrahmanyam, KS; Manna, AK; Pati, S. K.; Rao, CNR; A study of graphene decorated with metal nanoparticles. Chemical Physics Letters, 497, 70, 2010.

Kumar, S; Kamaraju, N; Vasu, KS; Nag, A; Sood, AK; Rao, CNR; Graphene analogue BCN: Femtosecond nonlinear optical susceptibility and hot carrier dynamics. **Chemical Physics Letters, 499,** 152, 2010.

Raidongia, K; Nag, A; Hembram, KPSS; Waghmare, UV; Datta, R; Rao, CNR; BCN: A Graphene Analogue with Remarkable Adsorptive Properties. **Chemistry-A European Journal, 16,** 149, 2010.

Jagadeesan, D; Eswaramoorthy, M; Functionalized Carbon Nanomaterials Derived from Carbohydrates. **Chemistry-An Asian Journal, 5,** 232, 2010.

Ghoshal, D; Maji, TK; Fabrication of supramolecular frameworks by tuning the binding site of a tripodal ligand with d^{10} metal ions: Interplay of covalent and non-covalent interactions in solid-state structure. **Journal of Chemical Sciences, 122,** 801, 2010.

Nagaraja, CM; Maji, TK; Rao, CNR; Synthesis and structures of Co(II), Ni(II), and Cu(II) coordination frameworks formed by a flexible 1,3-phenylenediacetic acid ligand. **Journal of Molecular Structure, 976,** 168, 2010.

Panchakarla, LS; Sundarayya, Y; Manjunatha, S; Sundaresan, A; Rao, CNR; On the Defect Origin of the Room-Temperature Magnetism Universally Exhibited by Metal-Oxide Nanoparticles. **ChemPhysChem, 11,** 1673, 2010.

Sarangi, SS; Zhao, W; Mueller-Plathe, F; Balasubramanian, S; Correlation between Dynamic Heterogeneity and Local Structure in a Room-Temperature Ionic Liquid: A Molecular Dynamics Study of [bmim][PF6]. **ChemPhysChem, 11,** 2001, 2010.

Gurunatha, KL; Mostafa, G; Ghoshal, D; Maji, TK; Single-crystal-to-single-crystal structural transformation in a three-dimensional bimetallic (4f-3d) supramolecular porous framework. **Crystal Growth & Design, 10,** 2483, 2010.

Heun, S; Radha, B; Ercolani, D; Kulkarni, GU; Rossi, F; Grillo, V; Salviati, G; Beltram, F; Sorba, L; Pd-Assisted Growth of InAs Nanowires. **Crystal Growth Design, 10,** 4197, 2010.

Hazra, A; Kanoo, P; Mohapatra, S; Mostafa, G; Maji, TK; A flexible supramolecular host with a crowned chair octameric water cluster and highly selective adsorption properties. **CrystEnggComm, 12,** 2775, 2010.

Mohapatra, S; Maji, TK; Facile synthesis of anion dependent versatile CuI and mixed-valent porous Cu^{I}/Cu^{II} frameworks. **Dalton Transactions, 39,** 3412, 2010.

Voggu, R; Shireen, A; Rao, CNR; One-step synthesis of high-purity fluorous-capped inorganic nanoparticles. **Dalton Transactions, 39,** 6021, 2010.

Nagaraja, CM; Behera, JN; Maji, TK; Pati, SK; Rao, CNR; Organically-templated Kagome compounds containing two transition metal ions. **Dalton Transactions, 39,** 6947, 2010.

Gupta, D; Mukhopadhyay, S; Narayan, KS; Fill factor in organic solar cells. **Solar Energy Materials and Solar Cells, 94,** 1309, 2010.

Mohapatra, S; Siddhanta, S; Kumar, DR; Narayana, C; Maji, TK; A facile bottom up approach for fabricating multifunctional silver nanorods. **European Journal of Inorganic Chemistry, 31,** 4969, 2010.

Kanoo, Prakash; Maji, TK; Construction of a 2D rectangular grid and 3D diamondoid interpenetrated frameworks and their functionalities by changing the second spacers. **European Journal of Inorganic Chemistry, 3762,** 2010.

Saini, G; Jacob, J; Senanayak, S; Narayan KS; Synthesis, characterization and OFET characteristics of 3,4-diaryl substituted poly(thienylene vinylene) derivatives. **Polymer Bulletin, 1007,** 1, 2010.

Kumar, P; Saha, S; Serrao, CR; Sood, AK; Rao, CNR; Temperature-dependent infrared reflectivity studies of multiferroic $TbMnO_3$: Evidence for spin-phonon coupling. **Pramana-Journal of Physics. 74,** 281, 2010.

Rao, CNR; Subrahmanyam, KS; Matte, HSSR; Abdulhakeem, B; Govindaraj, A; Das, B; Kumar, P; Ghosh, A; Late, Dattatray J.; A study of the synthetic methods and properties of graphenes. **Science and Technology of Advanced Materials, 11,** 054502, 2010.

Sagade, AA; Radha, B; Kulkarni, GU; Intricate nature of Pd nanocrystal–hydrogen interaction investigated using thermolysed Pd hexadecylthiolate films. **Sensors and Actuators B: Chemical, 149,** 345, 2010.

Kumar, N; Sundaresan, A; On the observation of negative magnetization under zero-field-cooled process. **Solid State Communications, 150,** 1162, 2010.

Vinod, K; Varghese, N; Sundaresan, A; Syamaprasad, U; Highly enhanced in-field critical current density of MgB_2 superconductor by combined addition of burned rice husk and nano Ho_2O_3. **Solid State Sciences, 12,** 610, 2010.

Jithesh, K; Govind; Kumar, M; Shivaprasad, SM; Clustering and layering of In adatoms on low and high index silicon surfaces: A comparative study. **Surface Science, 604,** 1972, 2010.

Subrahmanyam, KS; Kumar, P; Nag, A; Rao, CNR; Blue light emitting graphene-based materials and their use in generating white light. **Solid State Communications, 150,** 1774, 2010.

Late, DJ; Ghosh, A; Subrahmanyam, KS; Panchakarla, LS; Krupanidhi, SB; Rao, CNR; Characteristics of field-effect transistors based on undoped and B- and N-doped few-layer graphemes. **Solid State Communications, 150,** 734, 2010.

Panchakarla, LS; Govindaraj, A; Rao, CNR; Boron- and nitrogen-doped carbon nanotubes and graphene. **Inorganica Chimica ACTA, 363,** 4163, 2010.

Rao M; Ortiz, RP; Facchetti, A; Marks,TJ; Narayan, KS; Studies of Photogenerated Charge Carriers from Donor-Acceptor Interfaces in Organic Field Effect Transistors. Implications for Organic Solar Cells. **Journal of Physical Chemistry C, 114,** 20609, 2010.

Gautam, V; Bag, M; Narayan, KS; Dynamics of Bulk Polymer Heterostructure / Electrolyte Devices. **Journal of Physical Chemistry Letters, 1,** 3277, 2010.

Rao, CNR; Sood, AK; Voggu, R; Subrahmanyam, KS; Some Novel Attributes of Graphene. **Journal of Physical Chemistry Letters, 1,** 572, 2010.

Kumar, P; Saha, S; Muthu, DVS; Sahu, JR; Sood, AK; Rao, CNR; Raman evidence for orbiton-mediated multiphonon scattering in multiferroic $TbMnO_3$. **Journal of Physics-Condensed Matter, 22,** 115403, 2010.

Rao, CNR; Nag, A; Inorganic Analogues of Graphene. **European Journal of Inorganic Chemistry, 2010,** 4244, 2010.

Kanoo, P; Gurunatha, KL; Maji, TK; Versatile functionalities in MOFs assembled from the same building units: Interplay of structural flexibility, rigidity and regularity. **Journal of Materials Chemistry, 20,** 1322, 2010.

Mandal, P; Iyo, A; Tanaka, Y; Sundaresan, A; Rao, CNR; Structure, magnetism and giant dielectric constant of $BiCr_{0.5}Mn_{0.5}O_3$ synthesized at high pressures. **Journal of Materials Chemistry, 20,** 1646, 2010.

Samanta, SK; Pal, A; Bhattacharya, S; Rao, CNR; Carbon nanotube reinforced supramolecular gels with electrically conducting, viscoelastic and near-infrared sensitive properties. **Journal of Materials Chemistry, 20,** 6881, 2010.

Viswanathan, M.; Kumar, P. S. A.; Bhadram, V. S.; Narayana, C.; Bera, A. K.; Yusuf, S. M.; Influence of lattice distortion on the Curie temperature and spin-phonon coupling in $LaMn_{0.5}Ca_{0.5}O_3$. **Journal of Physics-Condensed Matter, 22,** 340006, 2010.

Varghese, N; Vinod, K; Shipra; Sundaresan, A; Syamaprasad, U; Burned Rice Husk: An Effective Additive for Enhancing the Electromagnetic Properties of MgB2 Superconductor. **Journal of The American Ceramic Society, 93,** 732, 2010.

Gomathi, A; Gopalakrishnan, K; Rao, CNR; Covalent functionalization of metal oxide and carbon nanostructures with polyoctasilsesquioxane (POSS) and their incorporation in polymer composites. **Materials Research Bulletin, 45,** 1894, 2010.

Samanta, SK; Gomathi, A; Bhattacharya, S; Rao, CNR; Novel Nanocomposites Made of Boron Nitride Nanotubes and a Physical Gel. **Langmuir, 26,** 12230, 2010.

Sharma, SN; Sharma, H; Singh, S; Mehra, RM; Singh, G; Shivaprasad, S. M.; Single pot synthesis of composition tunable CdSe-ZnSe (core-shell) and $Zn_xCd_{1-x}Se$ (ternary alloy) nanocrystals with high luminescence and stability. **Materials Research Innovations, 14,** 62, 2010.

Kurra, N; Scott, A; Kulkarni, GU; Electrocondensation and evaporation of attoliter water droplets: Direct visualization using AFM. **Nano Research, 3,** 307, 2010.

Radha, B; Kulkarni, GU; Micro- and Nanostripes of Self-assembled Au Nanocrystal Superlattices by Direct Micromolding. **Nano Research, 3,** 537, 2010.

Radha, B; Arif, M; Datta, R; Kundu, TK; Kulkarni, GU; Movable Au Microplates as Fluorescence Enhancing Substrates for Live Cells. **Nano Research, 3,** 738, 2010.

Rao, CNR; Voggu, R; Charge-transfer with graphene and nanotubes. **Materials Today, 13,** 34, 2010.

Bhuvana, T; Boley, W; Radha, B; Dolash, BD; Chiu, G; Bergstrom, D; Reifenberger, R; Fisher, TS; Kulkarni, GU; Inkjet printing of palladium alkanethiolates for facile fabrication of metal interconnects and surface-enhanced Raman scattering substrates. **Micro & Nano Letters, 5,** 296, 2010.

Scott, A; Gupta R; Kulkarni, GU; A Simple Water-Based Synthesis of Au Nanoparticle/PDMS Composites for Water Purification and Targeted Drug Release. **Macromolecular Chemistry and Physics, 211,** 1640, 2010.

Sharma, H; Sharma, SN; Singh, S; Mehra, NC; Singh, G; Shivaprasad, SM; Comparison of the properties of composition-tunable CdSe–ZnSe and $Zn_xCd_{1-x}Se$ nanocrystallites: Single- and double-pot synthesis approach. **Materials Chemistry and Physics, 124,** 670, 2010.

Voggu, R; Rao, KV; George, SJ; Rao, CNR; A Simple Method of Separating Metallic and Semiconducting Single-Walled Carbon Nanotubes Based on Molecular Charge Transfer. **Journal of The American Chemical Society, 132,** 5560, 2010.

John, NS; Raina, G; Sharma, A; Kulkarni, GU; Cellular network formation of hydrophobic alkanethiol capped gold nanoparticles on mica surface mediated by water islands. **Journal of Chemical Physics, 133,** 094704, 2010.

Raju, SG; Balasubramanian, S; Molecular dynamics simulation of model room temperature ionic liquids with divalent anions. **Indian Journal of Chemistry Section A-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, 49,** 721, 2010.

Asha, SK; Kolhe, N; Narayan, KS; Senanayak, S; n-Type Field Effect Transistors Based on Rigid Rod and Liquid Crystalline Alternating Copoly(benzobisoxazole) Imides Containing Perylene and/or Naphthalene. **Journal of Physical Chemistry B, 114,** 16694, 2010.

Voggu, R; Ghosh, Sandeep; Govindaraj, A; Rao, CNR; New Strategies for the Enrichment of Metallic Single-Walled Carbon Nanotubes. **Journal of Nanoscience And Nanotechnology, 10,** 4102, 2010.

Raju, SG; Balasubramanian, S; Role of Cation Symmetry in Intermolecular Structure and Dynamics of Room Temperature Ionic Liquids: Simulation Studies. **Journal of Physical Chemistry B, 114,** 6455, 2010.

Kumar, P; Panchakarla, LS; Bhat, SV; Maitra, U; Subrahmanyam, KS; Rao, CNR; Photoluminescence, white light emitting properties and related aspects of ZnO nanoparticles admixed with graphene and GaN. **Nanotechnology, 21,** 385701, 2010.

Tanaka, Y; Iyo, A; Tokiwa, K; Watanabe, T; Crisan, A; Sundaresan, A.; Topological structure of the inter-band phase difference soliton in two-band superconductivity. **Physica C, 470,** 1010, 2010.

Shipra, R; Takeya, H; Hirata, K; Sundaresan, A; Effects of Ni and Co doping on the physical properties of tetragonal $FeSe_{0.5}Te_{0.5}$ superconductor. **Physica C-Superconductivity and its applications, 470,** 528, 2010.

Maitra, U; Ghosh, S; Biswas, K; Rao, CNR; Scaling behavior of plasmon coupling in Au and ReO_3 nanoparticles incorporated in polymer matrices. **Physica Status Solidi-Rapid Research Letters, 4,** 169, 2010.

Sun, CQ; Nie, WY; Guang, Y; Mehta, BR; Shivaprasad, SM; Sun,Y; Pan, LK; Zhua, S; Interface quantum trap depression and charge polarization in the CuPd and AgPd bimetallic alloy catalysts. **Physical Chemistry Chemical Physics, 12,** 3121, 2010.

Raidongia, K; Gomathi, A; Rao, CNR; Synthesis and Characterization of Nanoparticles, Nanotubes, Nanopans, and Graphene-like Structures of Boron Nitride. **Israel Journal of Chemistry, 50,** 399, 2010.

Swain, D; Bhadram, VS; Gopal PK; Bhat, SV; Narayana, C; Rao, CN; Superionic Phase Transition in $KHSO_4$: A Temperature-Dependent Raman Investigation. **Journal of Physical Chemistry A, 114,** 10040, 2010.

Murugavel, S; Vaid, C; Bhadram VS; Narayana, C; Ion Transport Mechanism in Glasses: Non-Arrhenius Conductivity and Non-Universal Features. **Journal of Physical Chemistry B, 114,** 13381, 2010.

Radha, B; Sagade, AA; Kulkarni, GU; Flexible and Semitransparent Strain Sensors Based on 2 Micromolded Pd Nanoparticle-Carbon μ-Stripes. **ACS Applied Materials and Interfaces, 3,** 2173, 2011.

Narendra, K.; Sagade, A. A.; Kulkarni, G. U.; Ultrafast Direct Ablative Patterning of HOPG by Single Laser Pulses to Produce Graphene Ribbons. **Advanced Functional Materials, 21,** 3836, 2011.

Chitara, B; Panchakarla, LS; Krupanidhi, SB; Rao, CNR; Infrared Photodetectors Based on Reduced Graphene Oxide and Graphene Nanoribbons. **Advanced Materials, 23,** 5419, 2011.

Rao, KV; Datta, KKR; Eswaramoorthy, M; George, SJ; Light-Harvesting Hybrid Hydrogels: Energy Transfer Induced Amplified Fluorescence in Non-Covalently Assembled Chromophore-Organoclay Composites. **Angewandte Chemie International Edition, 50,** 1179, 2011.

Datta, KKR; Jagadeesan, D; Kulkarni, C; Kamath, A; Datta, R; Eswaramoorthy, M.; Observation of Pore-switching Behaviour in Porous Layered Carbon through Mesoscale Order-Disorder Transformation. **Angewandte Chemie International Edition, 50,** 3939, 2011.

Kesaria, M; Shivaprasad, SM; Nitrogen flux induced GaN nanostructure nucleation at misfit dislocations on Al_2O_3(0001). **Applied Physics Letters, 99,** 143105, 2011.

Roul, B.; Rajpalke, M. K.; Bhat, Thirumaleshwara N.; Kumar, M.; Kalghatgi, A. T.; Krupanidhi, S. B.; Kumar, N.; Sundaresan, A.; Experimental evidence of Ga-vacancy induced room temperature ferromagnetic behavior in GaN films. **Applied Physics Letters, 99,** 162512, 2011.

Das, AJ; Lafargue, C; Lebental, M; Zyss, J; Narayan, KS; Three-dimensional microlasers based on polymer fibers fabricated by electrospinning. **Applied Physics Letters, 99,** 263303, 2011.

Kumar, GVP; Rangarajan, N; Sonia, B; Deepika, P; Rohman, N; Narayana, C; Metal-coated magnetic nanoparticles for surface enhanced Raman scattering studies. **Bulletin of Materials Science, 34,** 207, 2011.

Kanoo, P; Haldar, R; Cyriac, ST; Maji, TK; Coordination driven axial chirality in a microporous solid assembled from an achiral linker via in situ C-N coupling. **Chemical Communications, 47,** 11038, 2011.

Hazra, A; Kanoo, P; Maji, TK; High heat of hydrogen adsorption and guest-responsive magnetic modulation in a 3D porous pillared-layer coordination framework. **Chemical Communications, 47,** 538, 2011.

Kanoo, P; Mostafa, G; Matsuda, R; Kitagawa, S; Maji, TK; A pillared-bilayer porous coordination polymer with a 1D channel and a 2D interlayer space, showing unique gas and vapor sorption. **Chemical Communications, 47,** 8106, 2011.

Kumar, N; Jagadeesan, D; Pillai, PB; Chacko, M; Eswaramoorthy, M; Sundaresan, A; Ferromagnetism in thin-walled hollow spheres of non-magnetic inorganic materials. **Chemical Physics Letters, 504,** 189, 2011.

Matte, HSSR; Subrahmanyam, KS; Rao, KV; George, SJ; Rao, CNR; Quenching of fluorescence of aromatic molecules by graphene due to electron transfer. **Chemical Physics Letters, 506,** 260, 2011.

Mohapatra, S; Kumar, RK; Maji, TK; Green synthesis of catalytic and ferromagnetic gold nanoparticles. **Chemical Physics Letters, 508,** 76, 2011.

Gopalakrishnan, K; Joshi, HM; Kumar, P; Panchakarla, LS; Rao, CNR; Selectivity in the photocatalytic properties of the composites of TiO_2 nanoparticles with B- and N-doped graphemes. **Chemical Physics Letters, 511,** 304, 2011.

Krishna, KS; Kumar, BVVS Pavan; Eswaramoorthy, M.; Nanopillar arrays of amorphous carbon nitride. **Chemical Physics Letters, 511,** 87, 2011.

Kulkarni, Chidambar; Reddy, Sandeep Kumar; George, SJ; Balasubramanian, S; Cooperativity in the stacking of benzene-1,3,5-tricarboxamide: The role of dispersion. **Chemical Physics Letters, 515,** 226, 2011.

Kumar, BVVS Pavan; Datta, KKR; Eswaramoorthy, M; Tuning the Nitrogen Content and Porosity of Nanostructured Carbon Nitride Using Aminoclay as a Reactive Template. **Chemistry Letters, 40,** 1154, 2011.

Maitra, U; Das, B; Kumar, N; Sundaresan, A; Rao, CNR; Ferromagnetism Exhibited by Nanoparticles of Noble Metals. **ChemPhysChem, 12,** 2322, 2011.

Das, B; Choudhury, B; Gomathi, A; Manna, AK; Pati, SK; Rao, CNR; Interaction of Inorganic Nanoparticles with Graphene. **ChemPhysChem, 12,** 937, 2011.

Gupta, R; Kulkarni, GU; Removal of Organic Compounds from Water by Using a Gold Nanoparticle–Poly(dimethylsiloxane) Nanocomposite Foam. **ChemSusChem, 4,** 737, 2011.

Kumar, N; Subrahmanyam, KS; Chaturbedy, P; Raidongia, K; Govindaraj, A; Hembram, KPSS; Mishra, AK; Waghmare, UV; Rao, CNR; Remarkable Uptake of CO_2 and CH_4 by Graphene-Like Borocarbonitrides, $B_xC_yN_z$. **ChemSusChem, 4,** 1662, 2011.

Dey, R; Haldar, R; Maji, TK; Ghoshal, D; Three-dimensional robust porous coordination polymer with schiff base site on the pore wall: Synthesis, single-crystal-to-single-crystal reversibility, and selective CO_2 adsorption. **Crystal Growth & Design, 11,** 3905, 2011.

Kesaria, M; Shetty S; Shivaprasad, SM; Evidence for Dislocation Induced Spontaneous Formation of GaN Nanowalls and Nanocolumns on bare C-Plane Sapphire. **Crystal Growth and Design, 11,** 4900, 2011.

Matte, HSSR; Plowman, B; Datta, Ranjan; Rao, CNR; Graphene analogues of layered metal selenides. **Dalton Transactions, 40,** 10322, 2011.

Nagaraja, CM; Kumar, N; Maji, TK; Rao, CNR; Amine-Templated Cobalt(II) Coordination Polymer Exhibiting Novel Magnetic Properties: Effect of Dehydration. **European Journal of Inorganic Chemistry, 2057,** 2011.

Dey, T; Khuntia, P; Mahajan, AV; Kumar, N; Sundaresan, A; ^{119}Sn NMR probe of magnetic fluctuations in SnO_2 nanoparticles. **European Physics Letters, 96,** 67008, 2011.

Moses, K; Panchakarla, LS; Matte, HSSR; Govindarao, B; Rao, CNR; Synthesis, characterization and spectroscopy of composites of graphene with CdSe and CdS nanoparticles. **Indian Journal of Chemistry Section A-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, 50,** 1239, 2011

Satapathi, S; Chattopadhyay, S; Bhar, K; Das, S; Kumar, RK; Maji, TK; Ghosh, BK; A new luminous hexacoordinated coordination polymer of cadmium(II) containing benzidine and dicyanamide as bridging units. **Inorganic Chemistry Communications, 14,** 632, 2011.

Kanoo, P; Sambhu, R; Maji, TK; Guest-specific double- or single-step adsorption in a flexible porous framework based on a mixed-ligand system. **Inorganic Chemistry, 50,** 400, 2011.

Kanoo, P; Ghosh, AC; Maji, TK; A Vanadium (VO^{2+}) Metal-organic framework: Selective vapor adsorption, magnetic properties, and use as a precursor for a polyoxovanadate. **Inorganic Chemistry, 50,** 5145, 2011.

Saha, R; Shireen, A; Shirodkar, SN; Singh, MS; Waghmare, UV; Sundaresan, A; Rao, CNR; Phase Transitions of $AlFeO_3$ and $GaFeO_3$ from the Chiral Orthorhombic ($Pna2_1$) Structure to the Rhombohedral R c Structure. **Inorganic Chemistry, 50,** 9527, 2011.

Bhar, K; Chattopadhyay, S; Khan, S; Kumar, RK; Maji, TK; Ribas, J; Ghosh, BK; Syntheses, structures and magnetic properties of mu(1,5) dicyanamide bridged coordination polymers of copper(II) and nickel(II) containing a tetradentate N-donor Schiff base. **Inorganica Chimica Acta, 370,** 492, 2011.

Rao, CNR; Subrahmanyam, KS; Matte, HSSR; Maitra, U; Moses, K; Govindaraj, A; Graphene: Synthesis, functionalization and properties. **International Journal of Modern Physics B, 25,** 4107, 2011.

Kumar, P; Kumar, M; Govind; Mehta BR; Shivaprasad, SM; Adsorption kinetics of low-dimensional Ga structures on Si(5 5 12)-2x1 trenched templates. **International Journal of Nanoscience, 1,** 117, 2011.

Vijaykumar, T; Kurra, N; Kulkarni, GU; Electron Beam Induced Carbonaceous Deposition as a Local Dielectric for CNT Circuits. **International Journal of Nanoscience, 10,** 1, 2011.

Bhuvana, T; Kulkarni, GU; Ultrafine ZnO Nanowires Grown on Patternable Pd Catalyst and Their Source-Energy Dependent Photoluminescence. **International Journal of Nanoscience, 10,** 699, 2011.

Pradhan, GK; Narayana, C; Rao, MN; Chaplot, SL; Pages, O; and et al,; The Phonon Percolation Scheme for Alloys: Extension to the Entire Lattice Dynamics and Pressure Dependence. **Japanese Journal of Applied Physics, 50,** 05FE02, 2011.

Mukhophadyay, S; Voggu, R; Vidhydhiraja, N; Rao, CNR; Narayan, KS; Lateral Photocurrent Scanning of Donor and Acceptor Polymers on Graphene Coated Substrates. **Japanese Journal of Applied Physics, 50,** 061602, 2011.

Kuyyalli, J; Tangi, M; Shivaprasad, SM; Dependence of crystal orientation and bandgap on substrate temperature of molecular-beam epitaxy grown InN on bare Al_2O_3 (0001). **Journal Applied Physics, 109,** 093513, 2011.

Vijay V; Arun D; Narayan, KS; In-situ Studies of Strain Dependent Transport Properties of Conducting Polymers on Elastomeric Substrates. **Journal of Applied Physics, 109,** 084525, 2011.

Nair, HS; Swain, D; Hariharan, N; Adiga, S; Narayana, C; Elzabeth, S; Griffiths phase-like behavior and spin-phonon coupling in double perovskite Tb_2NiMnO_6. **Journal of Applied Physics, 110,** 123919, 2011.

Reddy, SK; Kulkarni, CH; Balasubramanian, S; Theoretical investigations of candidate crystal structures for beta-carbonic acid. **Journal of Chemical Physics, 134,** 124511, 2011.

Das, AJ; Mukhopadhyay, S; Narayan, KS; Characteristic noise features in light transmission across membrane protein undergoing photocycle. **Journal of Chemical Physics, 134,** 175101, 2011.

Haldar, R; Maji, TK; A two-fold interpenetrated flexible bi-pillared-layer framework of Fe(II) with interesting solvent adsorption property. **Journal of Chemical Sciences, 123,** 883, 2011.

Chaturbedy, P; Matte, HSSR; Voggu, R; Govindaraj, A; Rao, CNR; Self-assembly of C(60), SWNTs and few-layer graphene and their binary composites at the organic-aqueous interface. **Journal of Colloid and Interface Science, 360,** 249, 2011.

Kesaria, M; Shetty S; Shivaprasad, SM; Spontaneous formation of GaN nanostructures by molecular beam epitaxy. **Journal of Crystal Growth, 326,** 191, 2011.

Hodson, SL; Bhuvana, T; Kulkarni, GU; Fisher, TS; Palladium Thiolate Bonding of Carbon Nanotube Thermal Interfaces. **Journal of Electronic Packaging, 33,** 020907, 2011.

Rao, KV; Mohapatra, S; Kulkarni, C; Maji, TK; George, SJ; Extended phenylene based microporous organic polymers with selective carbon dioxide adsorption. **Journal of Materials Chemistry, 21,** 12958, 2011.

Shireen, A; Saha, R; Mandal, P; Sundaresan, A; Rao, CNR; Multiferroic and magnetodielectric properties of the $Al_{1-x}Ga_xFeO_3$ family of oxides. **Journal of Materials Chemistry, 21,** 57, 2011.

Kundu, PP; Kumar, GVP; Mantelingu, K; Kundu, TaK; Narayana, C; Raman and surface enhanced Raman spectroscopic studies of specific, small molecule activator of histone acetyltransferase p300. **Journal of Molecular Structure, 999,** 10, 2011.

Radha, B; Sagade, AA; Gupta, R; Kulkarni, GU; Direct Micromolding of Pd -Stripes for Electronic Applications. **Journal of Nanoscience and Nanotechnology, 11,** 1, 2011.

Kurra, N; Vijaykumar, T; Kulkarni, GU; CNT Manipulation: Inserting a Carbonaceous Dielectric Layer Beneath Using Electron Beam Induced Deposition. **Journal of Nanoscience and Nanotechnology, 11,** 1025, 2011.

Das, S; Bhadram, VS; Narayana, C; Bhattacharyya, AJ; Brillouin Scattering Investigation of Solvation Dynamics in Succinonitrile-Lithium Salt Plastic Crystalline Electrolytes. **Journal of Physical Chemistry B, 115,** 12356, 2011.

Sarangi, SS; Reddy, SK; Balasubramanian, S; Low Frequency Vibrational Modes of Room Temperature Ionic Liquids. **Journal of Physical Chemistry B, 115,** 1874, 2011.

Mukhopadhyay, S; Ramachandra, S; Narayan, KS; Direct Observation of Charge Generating Regions and Transport Pathways in Bulk Heterojunction Solar Cells with Asymmetric Electrodes Using near Field Photocurrent Microscopy. **Journal of Physical Chemistry C, 115,** 17184, 2011.

Mallikarjuna Rao, K; Bhuvana, T; Radha, B; Narendra, K; Vidhyadhiraja NS; Kulkarni, GU; Metallic Conduction in NiS_2 Nanocrystalline Structures. **Journal of Physical Chemistry C, 21,** 1046, 2011.

Late, Dattatray J; Maitra, U; Panchakarla, LS; Waghmare, UV; Rao, CNR; Temperature effects on the Raman spectra of graphenes: dependence on the number of layers and doping. **Journal of Physics-Condensed Matter, 23,** 055303, 2011.

Sundarayya, Y; Mandal, P; Sundaresan, A; Rao, CNR; Mossbauer spectroscopic study of spin reorientation in Mn-substituted yttrium orthoferrite. **Journal of Physics-Condensed Matter, 23,** 436001, 2011.

Saha, R; Shireen, A; Shirodkar, SN; Waghmare, UV; Sundaresan, A; Rao, CNR; Effect of Cr and Mn ions on the structure and magnetic properties of $GaFeO_3$: Role of the substitution site. **Journal of Solid State Chemistry, 184,** 2353, 2011.

Kumar, N; Raidongia, K; Mishra, AK; Waghmare, UV; Sundaresan, A; Rao, CNR; Synthetic approaches to borocarbonitrides, BC_xN (x=1-2). **Journal of Solid State Chemistry, 184,** 2902, 2011.

Saha, R; Shireen, A; Bera, AK; Shirodkar, SN; Sundarayya, Y; Kalarikkal, N; Yusuf, SM; Waghmare, UV; Sundaresan, A; Rao, CNR; Structure and magnetic properties of the $Al_{1-x}Ga_xFeO_3$ family of oxides: A combined experimental and theoretical study. **Journal of Solid State Chemistry, 184,** 494, 2011.

Varghese, N; Vinod, K; Rahul, S; Anees, P; Devadas, KM; Thomas, S; Shipra; Sundaresan, A; Roy, SB; Syamaprasad, U; Effect of Carbon Substitution on the Superconducting Properties of Nanocarbon-, Nanodiamond- and Nano-SiC-Doped MgB_2. **Journal of The American Ceramic Society, 94,** 1133, 2011.

Radha, B; Kiruthika, S; Kulkarni, GU; Metal Anion-Alkyl Ammonium Complexes as Direct Write Precursorsto Produce Nanopatterns of Metals, Nitrides, Oxides, Sulfides And Alloys. **Journal of the American Chemical Society, 133,** 12706, 2011.

Gautam, V; Bag, M; Narayan, KS; Single-Pixel, Single-Layer Polymer Device as a Tricolor Sensor with Signals Mimicking Natural Photoreceptors. **Journal of The American Chemical Society, 133,** 17942, 2011.

Dlamini, LN; Krause, RW; Kulkarni, GU; Durbach, SH; Synthesis and characterization of titania based binary metal oxide nanocomposite as potential environmental photocatalysts. **Materials Chemistry and Physics, 129,** 406, 2011.

Varghese, N; Rao, CNR; Magnetic nanofilms of nickel prepared at the liquid-liquid interface. **Materials Research Bulletin, 46,** 1500, 2011.

Kesaria, M; Shetty S; Shivaprasad, SM; Transformation of c-oriented nanowall network to a flat morphology in GaN films on c-plane sapphire. **Materials Research Bulletin, 46,** 1811, 2011.

Kumar, N; Sundaresan, A; Rao, CNR; Rare earth niobium oxynitrides, LnNbON(2-δ) (Ln = Y, La, Pr, Nd, Gd, Dy): Synthesis, structure and properties. **Materials Research Bulletin, 46,** 2021, 2011.

Rao, CNR; Subrahmanyam, KS; Matte, HSSR; Govindaraj, A; Graphene: synthesis, functionalization and properties. **Modern Physics Letters B, 25,** 427, 2011.

Kulkarni, GU; Radha, B; Metal nanowire grating patterns. **Nanoscale, 2,** 2035, 2010.

Kumar, P; Panchakarla, LS; Rao, CNR; Laser-induced unzipping of carbon nanotubes to yield graphene nanoribbons. **Nanoscale, 3,** 2127, 2011.

Sasidharan, A; Panchakarla, LS; Chandran, P; Menon, D; Nair, S; Rao, CNR; Koyakutty, M; Differential nano-bio interactions and toxicity effects of pristine versus functionalized graphene. **Nanoscale, 3,** 2461, 2011.

Rout, C. S.; Kumar, A.; Kumar, N.; Sundaresan, A.; Fisher, T. S.; Room-temperature ferromagnetism in graphitic petal arrays. **Nanoscale, 3,** 900, 2011.

Kurra, N; Prakash, G; Basavaraja, S; Fisher, TS; Kulkarni, GU; Reifenberger, RG; Charge storage in mesoscopic graphitic islands fabricated using AFM bias lithography. **Nanotechnology, 22,** 245302, 2011.

Karimi-Varzaneh, HA; Mueller-Plathe, F; Balasubramanian, S; Carbone, P; Studying long-time dynamics of imidazolium-based ionic liquids with a systematically coarse-grained model. **Physical Chemistry Chemical Physics, 12,** 4714, 2010.

Sarangi, SS; Raju, SG; Balasubramanian, S; Molecular dynamics simulations of ionic liquid-vapour interfaces: effect of cation symmetry on structure at the interface. **Physical Chemistry Chemical Physics, 13,** 2714, 2011.

Pradhan, GK; Narayana, C; Pages, O; Breidi, A; Souhabi, J; Postnikov, AV; Deb, SK; Firszt, F; Paszkowicz, W; Shukla, A; Hassan, F El Haj.; Pressure-induced phonon freezing in the $Zn_{1-x}Be_xSe$ alloy: A study via the percolation model. **Physical Review B, 81,** 115207, 2010.

Bera, MK; Sanyal, MK; Yang, L; Biswas, K; Gibaud, A; Rao, CNR; Small-angle x-ray scattering study of the aggregation of gold nanoparticles during formation at the toluene-water interface. **Physical Review B, 81,** 115415, 2010.

Bag, M; Narayan, KS; Universality in the intensity-modulated photocurrent in bulk-heterojunction polymer solar cells. **Physical Review B, 82,** 075308, 2010.

Mandal, P; Sundaresan, A; Rao, CNR; Iyo, A; Shirage, PM; Tanaka, Y; Simon, Ch; Pralong, V; Lebedev, OI; Caignaert, V; Raveau, B; Temperature-induced magnetization reversal in $BiFe_{0.5}Mn_{0.5}O_3$ synthesized at high pressure. **Physical Review B, 82,** 100416, 2010.

Gopal, PK; Kumar, A; Deb, SK; Waghmare, UV; Narayana, C; Elastic and structural instability of cubic Sn_3N_4 and C_3N_4 under pressure. **Physical Review B, 82,** 144112, 2010.

Choudhury, D; Mukherjee, S; Mandal, P; Sundaresan, A; Waghmare, UV; Bhattacharjee, S; Mathieu, R; Lazor, P; Eriksson, O; Sanyal, B; Nordblad, P; Sharma, A; Bhat, SV; Karis, O; Sarma, DD; Tuning of dielectric properties and magnetism of $SrTiO_3$ by site-specific doping of Mn. **Physical Review B, 84,** 125124, 2011.

Mandal, P; Bhadram, VS; Sundarayya, Y; Narayana, C; Sundaresan, A; Rao, CNR; Spin-Reorientation, Ferroelectricity, and Magnetodielectric Effect in $YFe_{1-x}Mn_xO_3(0.1\leq x \leq 0.40)$. **Physical Review Letters, 107,** 137202, 2011.

Galkin, KN; Kumar, M; Shivaprasad, SM; Galkin, NG; The model of the magnesium silicide phase (2/3√3×2/3√3)-R30° on Si(111). **Physics Procedia, 11,** 47, 2011.

Galkin, KN; Kumar, M; Shivaprasad, SM; Galkin, NG; AES and EELS study of desorption of magnesium silicide films on Si(111). **Physics Procedia, 11,** 51, 2011.

Satapathi, S; Das, S; Bhar, K; Kumar, RK; Maji, TK; Ghosh, BK; Syntheses, structures and luminescence behavior of mono- and dinuclear complexes of type $[M(L)(NCS)_2]_n$ [M = Zn/Hg, n=1; M = Cd, n=2; L = (N,N-diethyl,N'-(pyridin-2-yl)benzylidene)ethane-1,2-diamine]: Variation of coordination matrices and nuclearities with the change of congeneric metal ions. **Polyhedron, 30,** 387, 2011.

Heun, S; Radha, B; Ercolani, D; Kulkarni, GU; Rossi, F; Grillo, V; Salviati, G; Beltram, F; Sorba, L; Coexistence of Vapor-Liquid-Solid and Vapor-Solid-Solid Growth Modes in Pd-Assisted InAs Nanowires. **Small, 6,** 1935, 2010.

Das, S; Senanayak, SP; Bedi, A; Narayan, KS; Zade, SS; Synthesis and charge carrier mobility of a solution-processable conjugated copolymer based on cyclopenta[c]thiophene. **Polymer, 52,** 5780, 2011.

Subrahmanyam, KS; Kumar, P; Maitra, U; Govindaraj, A; Hembram, KPSS; Waghmare, UV; Rao, CNR; Chemical storage of hydrogen in few-layer graphene. **Proceedings of The National Academy of Sciences of The United States of America, 108,** 2674, 2011.

Verma, A; Sharma, A; Kulkarni, GU; Ultrafast Large-Area Micropattern Generation in Nonabsorbing Polymer Thin Films by Pulsed Laser Diffraction. **Small, 7,** 758, 2011.

Bhargavi, R.; Nair, Geetha G.; Prasad, S. Krishna; Kumar, N.; Sundaresan, A.; Enhanced Frank elasticity and storage modulus in a diamagnetic liquid crystalline ferrogel. **Soft Matter, 7,** 10151, 2011.

Bhat, SV; Govindaraj, A; Rao, CNR; Hybrid solar cell based on P3HT-ZnO nanoparticle blend in the inverted device configuration. **Solar Energy Materials and Solar Cells, 95,** 2318, 2011.

Kumar, P; Kuyyalli, J; Kumar, M; Shivaprasad, SM; A superstructural 2D-phase diagram for Ga on the Si(111)-7x7 system. **Solid State Communications, 151,** 1758, 2011.

Kumar, P.; Kumar, M.; Mehta, B. R.; Shivaprasad, S. M.; Ga-induced restructuring of Si(5 5 12) – 2 × 1 reconstructed surface at room temperature. **Surface Science, 605,** 1426, 2011.

Chauhan, AKS; Govind, JK; Shivaprasad, SM; Adsorption/desorption kinetics of Na atoms on reconstructed Si (111)-7 x 7 surface. **Thin Solid Films 519,** 1012, 2010.

Raidongia, K; Hembram, KPSS; Waghmare, UV; Eswaramoorthy, M.; Rao, CNR; Synthesis, Structure, and Properties of Mesoporous B/C/N Microspheres. **Zeitschrift Fur Anorganische Und Allgemeine Chemie, 636,** 30, 2010.

ENGINEERING MECHANICS UNIT

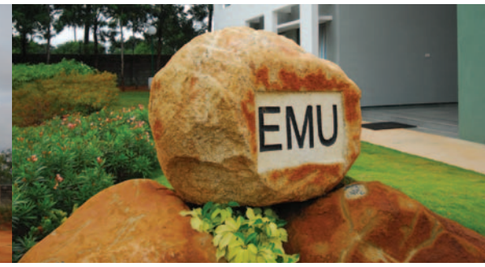
Sahu, Kirti Chandra; Govindarajan, Rama, Spatio-temporal linear stability of double-diffusive two-fluid channel flow. **Physics of Fluids, 24,** 054103, 2012.

Majumder, A; Kariwala, V.; Ansumali, S; Rajendran, A, Lattice Boltzmann method for multi-dimensional population balance models in crystallization. **Chemical Engineering Science, 70,** 121134, 2012.

Majumder, A; Kariwala, V; Ansumali, S; Rajendran, A, Lattice Boltzmann method for population balance equations with simultaneous growth, nucleation, aggregation and breakage. **Chemical Engineering Science, 69,** 316-328, 2012.

Vinod, N; Govindarajan, Rama, Secondary instabilities in incompressible axisymmetric boundary layers: effect of transverse curvature. **Journal of Fluids Engineering, ASME. 134(2),** 024503, 2012.

Kumar,Nitin; Majumdar,Sayantan; Sood, Aditya; Govindarajan,Rama; Ramaswamy, Sriram; Sood, AK, Oscillatory settling in wormlike-micelle solutions: bursts and a long time scale. **Soft Matter, 8,** 4310-4313, 2012.



Ponnulakshmi, VK; Mukund, V; Singh, DK; Sreenivas, KR; Subramanian, G; Hypercooling in the noc1 turnal boundary layer: Broadband emissivity schemes and beyond. **Journal of Atmospheric Sciences, 2012.**

Dasgupta, Ratul; and Govindarajan,Rama; The hydraulic jump and the shallow water equations. **International Journal of Advances in Engineering Sciences and Applied Mathematics, Special Issue, 3 (1-4),** 126-130, 2012.

Sudhakar, Subudhi; Sreenivas, KR; Arakeri, Jaywant H; Real source-sink pair. **International Journal of Heat and Mass Transfer 55,** 1650□1660, doi:10.1016/j.ijheatmasstransfer.2011.11.021, 2012.

Sudhakar Subudhi, Sreenivas, KR; Arakeri, Jaywant H; Natural ventilation in a model room. **Journal of Thermal Science and Engineering Applications, 4,** 011003, 2012.

Alam, Meheboob; Shukla, P., Origin of subcritical shear-banding instability in a dense two-dimensional sheared granular fluid. **Granular Matter 14,** 221-227, 2012.

Alam, Meheboob, Non-model stability and optimal perturbation in unbounded granular shear flow: three-dimentionalityand particle spin. **Progress of Theoretical Physics Supplement 195,** 78-100, 2012.

Eshnis, P; vendoer Welle, K; Alam, Meheboob; Lohse, D, Buoyancy driven convection in vertically shaken granular matter: experiments, numerics and theory. **Granular Matter 14,** 2012.

Sahu, Kirti Chandra; Govindarajan, Rama; Linear stability of double diffusive two-fluid channel flow. **Journal of Fluid Mechanics, 687,** 529-539, 2011.

Sumesh, PT; Govindarajan, Rama; Minimum energy shapes of one-side-pinned static drops on inclined surfaces. **Physical Review E, 84,** 046304, 2011.

Dixit, Harish N; Govindarajan, Rama; Stability of a vortex in radial density stratification: role of wave interactions. **Journal of Fluid Mechanics, 679,** 582- 615, 2011.

Swaminathan, Gayathri; Sahu, Kirti Chandra; Sameen, A; Govindarajan, Rama; Global instabilities in diverging channel flows. **Theoretical and Computational Fluid Dynamics, 25,** 53-64, 2011.

Srikanth, T; Dixit, Harish N; Rao, Tatavarti; Govindarajan, Rama; Vortex shedding patterns, their competition, and chaos in flow past inline oscillating rectangular cylinders. **Physics of Fluids 23,** 073603, 2011.

Subramanian, Ganesh; and Nott, Prabhu R; The fluid dynamics of swimming microorganisms and cells. **IISc Journal, 91(3),** 283-313, July-Sept. 2011.

Gayen, B; Alam, Meheboob; Effect of Coulomb friction on orientational correlation and velocity distribution functions in a sheared dilute granular gas. **Physical Review E, 84,** 021304, 2011.

Koch, DL; and Subramanian, G; Collective hydrodynamics of swimming micro-organisms: Living fluids. **Annual Reviews of Fluid Mechanics, 43,** 637-659, 2011.

Mynam, M; Sunthar, P; Ansumali, S; Efficient Lattice Boltzmann Algorithm for Brownian Suspensions. **Philosophical Transactions of the Royal Society A, 369,** 2237-2245, 2011.

Prasianakis, N; Ansumali, S; Microflow Simulations via the Lattice Boltzmann Method. **Communications in Computational Physics, 9,** 1128-1136, 2011.

Singh, OP; Ranjan, D; Srinivasan, J; Sreenivas, KR; A study of basalt fingers using experiments and numerical simulation in double-diffusive systems. **Journal Geography and Geology, 3(1),** 2011.

Narasimha, R; Diwan, Sourabh Suhas; Duvvuri, Subrahmanyam; Sreenivas, KR; Bhat, GS; Laboratory simulations show diabatic heating drives cumulus-cloud evolution and entrainment. **Proceedings of the National Academy of Sciences (PNAS),** 108:39. 16164–16169, 2011

25. Narasimha, R; Diwan, SS; Duvvuri, S; Sreenivas, KR; and Bhat, GS; Laboratory simulations show diabatic heating drives cumulus-cloud evolution and entrainment. **Proceedings of National Academy of sciences, PNAS, 2011,** doi:10.1073/pnas.1112281108

Narasimha, R; Kosambi and Proper Orthogonal Decomposition. **Resonance 16,** 574-581, 2011.

Ansumali, S; Mean-Field Model beyond Boltzmann-Enskog Picture for Dense Gases. **Communications in Computational Physics, 9,** 1106-1116, 2011.

Singh, Shiwani; Subramanian, Ganesh; and Ansumali, Santosh; A Lattice Boltzmann method for dilute polymer solutions. **Philosophical transactions of the Royal Society A, 369,** 2301-2310, 2011.

Shreyas, JV; Devranjan, S; and Sreenivas, KR; Aerodynamics of Bird and Insect Flight. **Journal of the Indian Institute of Science, 91:3,** 315-327, July-Sept. 2011.

Shukla, P; Alam, Meheboob; Weakly nonlinear theory of shear-banding instability in granular plane Couette flow: analytical solution, comparison with numerics and bifurcation. **Journal of Fluid Mechanics, 666,** 204–253, 2011.

Shukla, P; Alam, Meheboob; Nonlinear stability and patterns in granular plane Couette flow: Hopf and pitchfork bifurcations, and evidence for resonance. **Journal of Fluid Mechanics, 672,** 147-195, 2011.

Simha, RV; Arakeri, JH; Usha, S; and Sreenivas, KR; Earth Air Tunnel and comfort cooling (and heating) Part-2. **Air conditioning and refrigeration journal, 102-109,** 2011.

Smith, KC; Fisher, TS; Alam, Meheboob; Isostaticity of constraints in amorphous jammed systems of soft frictionless Platonic solids. **Physical Review E (Rapid Communication), 84,** 030301, 2011.

Diwan, Sourabh S; Narasimha, Roddam; Bhat, GS; and Sreenivas, KR Laboratory Studies of Anomalous Entrainment in Cumulus Cloud Flows. **Journal of Physics: Conference Series, 318,** 072014, doi:10.1088/1742-6596/318/7/072014, 2011.

Diwan, Sourabh S; Narasimha, R; Bhat, GS; and Sreenivas, KR; Laboratory Studies of Anomalous Entrainment in Cumulus Cloud Flows. Proceedings of 13th European Turbulence Conference (ETC13). **Journal of Physics: Conference Series 318,** 072014, 2011. doi:10.1088/1742-6596/318/7/072014

Subramanian, G; and Koch, DL; The influence of the inertially dominated outer region on the rheology of a dilute suspension of low-Reynolds-number drops and particles. **Journal of Fluid Mechanics, 674,** 307-358, 2011.

Subramanian, G; Koch, DL; and Fitzgibbon, Sean R; The stability of a homogeneous suspension of chemotactic bacteria. **Physics of Fluids, 23,** 041901, 2011.

Abbas, A; and Ansumali, S; Global potential of rice husk as a renewable feedstock for ethanol biofuel production. **BioEnergy Research, 3,** 328-334 (2010)

Majumder, A; Kariwala, V; Ansumali, S; and Rajendran, A; Entropic Lattice Boltzmann method for crystallization process. **Chemical Engineering Science, 69,** 3928-3936, 2010.

Majumder, A; Kariwala, V; Ansumali, S; and Rajendran, A; Fast High Resolution Method for Solving Multi-dimensional Population Balances in Crystallization. **Industrial & Engineering Chemistry Research, 49,** 3862-3872, 2010.

Alam, Meheboob; Chikkadi, V; Velocity distribution function and correlations in a granular Poiseuille flow, **Journal of Fluid Mechanics, 653,** 175–219, 2010.

Eshuis, P; van der Meer, D; Alam, Meheboob; van Gerner, HJ; van der Welle, K; Lohse, D; Onset of Convection in Strongly Shaken Granular Matter. **Physical Review Letters, 104,** 038001, 2010.

Subramanian, Ganesh; Viscosity-enhanced bio-mixing of the oceans. **Current Science, 98(8),** 1103-1108, 2010.

Subramanian, Ganesh; Wading through Bachelor's book: book review. **Resonance - journal of science education, 15(4),** 363-383, 2010.

Mukund, V; Ponnulakshmi; Singh, VK; Subramanian, DK; G; and Sreenivas, KR; Hyper-cooling in the nocturnal boundary layer: the Ramdas paradox. **Physica Scripta, T142,** DI 10.1088/0031-8949/2010/T142/014041, 2010

Mukund, V, Ponnulakshmi, VK; Dheeraj, KS; Subramanian, G; and Sreenivas, KR, Hyper-cooling in the nocturnal boundary layer – the Ramdas paradox. **Physica Scripta, T142,** 014041, 2010.

Narasimha, R; Bhattacharyya, Subarna; A wavelet cross-spectral analysis of Solar-ENSO-rainfall connections in the Indian Monsoons. **Applied and Computational Harmonic Analysis 28,** 285-295, 2010. doi:10.1016/j.acha.2010.02.005.

Suryanarayanan, Saikishan; and Narasimha, R; Point-Vortex Simulations Reveal Universality Class in Growth of 2D Turbulent Mixing Layers, **arXiv:1008.2876v1** [physics.flu-dyn], 2010.

Simha, RV; Arakeri, JH; Usha, S; and Sreenivas, KR; Earth Air Tunnel and comfort cooling (and heating) Part-1, **Air conditioning and refrigeration journal, 48-60,** 2010.

Smith, KC; Alam, Meheboob; Fisher, TS; Athermal jamming of soft frictionless Platonic solids. **Physical Review E, 82,** 051304, 2010.

Raja, Vivek R; Subramanian, G; and Koch, DL; Inertial effects on the rheology of a dilute emulsion. **Journal of Fluid Mechanics, 646,** 255-296, 2010.

Yudistiawan, WP; Kwak, SK; Patil, DV; and Ansumali, S; Higher-order Galilean-invariant lattice Boltzmann model for microflows: Single-component gas. **Physical Review E, 82,** 046701, 2010.

Dasgupta, Ratul; & Govindarajan, Rama; Non-similar solutions of the viscous shallow water equations governing weak hydraulic jumps. **Physics of Fluids, 22,** 112108, 2010.

Dixit, Harish N; & Govindarajan, Rama; Vortex-induced instabilities and accelerated collapse due to inertial effects of density stratification. **Journal of Fluid Mechanics 646,** 415 -439, 2010.

Sumesh, PT; & Rama, Govindarajan; The possible equilibrium shapes of static pendant drops. **Journal of Chemical Physics 133,** 144707, 2010.

Bale, Rahul; & Govindarajan, Rama; Transient growth and why we should care about it. **Resonance, 15(5),** 441-457, 2010.

Conference Proceedings

Vybhav, GR; Sourabh, S; Diwan, Sreenivas, KR; Narasimha, R; Venkatakrishnan, L; and Suriyanarayanan, P; Laboratory simulation of the life-cycle of a cumulus congestus cloud. **Proceedings of International conference on "Opportunities and Challenges in Monsoon Prediction in a Changing Climate" (OCHAMP-2012),** Pune, India, 21-25 February 2012.

Ravichandran, S; Govindarajan, Rama; and Narasimha, Roddam; Inertial particles in leap-frogging vortex-pair flow. **IUTAM Symposium on mobile particulate systems, 2012.**

Venkataraman, Divya; Bottaro, Alessandro; Govindarajan, Rama; Flow control via porous coating of compliant actuators: a simple interactive model Flow control via porous coating of compliant actuators: a simple interactive model. **Proceedings of IUTAM Symposium on Bluff Body Wakes, 2011.**

Rakshith, BR; Deshpande, SM; Praveen, C; Narasimha, R; Assessment of lifting-line theory optimization of turboprop wings in tractor configuration using Euler code. **Proceedings of Symposium of Applied Aerodynamics and Design of Aerospace Vehicles, pp 564,** 2011.

Alam, Meheboob; Shukla, P; Dynamics and patterns in sheared granular fluid: Order parameter description and bifurcation scenario. **Proceedings of the Workshop on Nonequilibrium Dynamics in Astrophysics and Material Science, 1-3 November,** 2011, Kyoto University, Kyoto, Japan.

Alam, Meheboob; Shukla, P; Exact order parameter theory for patterns and mode interactions in driven granular systems. **Proceedings of the SIAM Conference on Dynamical Systems,** 22-26 May 2011, Snowbird, Salt-Lake City, Utah, USA.

Gupta, V; Alam, Meheboob; Constitutive relations for a granular fluid of smooth inelastic hard spheres, till Burnett order. **Bulletin of the American Physical Society,** 21-25 March 2011, Dallas, Texas, USA.

Shukla, P; Alam, Meheboob; Shear banding instability and patterns in granular plane Couette flow. **Bulletin of the American Physical Society,** 21-25 March 2011, Dallas, Texas, USA.

Singh, DK; Ponnulakshmi, VK; Subramanian, G; and Sreenivas, KR; Experimental studies to characterize radiation forcing by atmospheric aerosols. **Proceedings of the 21st, National and 10th ISHMT-ASME Heat and Mass Transfer Conference,** December 27-30, 2011, IIT Madras, India, ISHMT-IND-07-004, 2011.

Sreenivas, KR; Singh, DK; Ponnulakshmi, VK; Subramanian, G; Experimental Characterization of Radiation Forcing due to Atmospheric Aerosols. **Bulletin of the American Physical Society 64th Annual Meeting of the APS Division of Fluid Dynamics,** Volume 56, Number 18, November 20–22, 2011.

Ponnulakshmi, VK; Singh, DK; Sreenivas, KR; and Subramanian, G; The role of aerosol in the laboratory simulation of Ramdas layer. **Proceedings of the 21st, National and 10th ISHMT-ASME Heat and Mass Transfer Conference,** December 27-30, 2011, IIT Madras, India, 2011.

Alam, Meheboob; Shukla, P; Order parameter theory for patterns in granular shear flow, **Proceedings of the Workshop on Recent Progress in Physics of Dissipative Particles,** 24-26 November, 2010, Kyoto University, Kyoto, Japan.

Shukla, P; Alam, Meheboob; Nonlinear stability, bifurcation and resonance in granular plane Couette flow. **Bulletin of 63rd Annual Meeting of the APS's Division of Fluid Dynamics,** 21-23 November 2010, Long Beach, California, USA.

Shukla, P; Alam, Meheboob; Nonlinear stability of granular plane Couette flow: Shear banding. **Bulletin of 63rd Annual Meeting of the APS's Division of Fluid Dynamics,** 21-23 November 2010, Long Beach, California, USA.

Alam, Meheboob; Shukla, P; Nonlinear stability, bifurcation and patterns in granular plane Couette flow. **Proceedings of the 8th Euromech Fluid Mechanics Conference,** 13-16 September 2010, Bad Reichenhall, Germany.

Sreenivas, KR; Vivek, NP; and Arakeri, JH; An Experimental Study of Mantle Like Convection. **7th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics (HEFAT-2010),** Antalya, Turkey. 19-21 July 2010

Vivek, NP; and Arakeri, JH; Sreenivas, KR; The Role of Viscosity Contrast on the Plume Structure and Dynamics in High Rayleigh Number Convection. **[LH.00007] 63rd Annual Meeting of the APS Division of Fluid Dynamic,** Long Beach, California, USA, 21-23, November, 2010.

Narasimha, R; Diwan, SS; Subrahmanyam, D; Sreenivas, KR; Bhat, GS; Laboratory simulations of cumulus cloud flows explain the entrainment anomaly [MG.00006]. **63rd Annual Meeting of the APS Division of Fluid Dynamic,** Long Beach, California, USA, 21-23, November, 2010.

Prakash, Vivek N; Sreenivas, KR; and Arakeri, J H; Plume structures at different viscosity ratios across the bottom boundary layer, **(contesting POSTER for the APS DFD Gallery of fluid motion-2010).**

Siddharth, K; Dwarakanath, T; and Sreenivas, KR; Experiments and numerical simulations for the quantification of lift in flapping flight, **International Conference On Intelligent Unmanned Systems Bali,** Indonesia, NOV 3-5, 2010.

Singh, D K; Ponnulakshmi, VK; Mukund, V; Subramanian, G; Sreenivas, KR; Surface Aerosols, Radiation Forcing and Vertical Temperature Profiles AAAR. **29th Annual Conference, Oregon Convention Center,** Portland, October 25-29, 2010.

Narasimha, R; Diwan, S; Subrahmanyam, D; Sreenivas, KR, Bhat, GS; Entrainment in Laboratory Simulations of Cumulus Cloud Flows. **AGU Fall Meeting Abstracts, 1,** 0127, 2010.

Narasimha, R; Diwan, S; Subrahmanyam, D; Sreenivas, KR, and Bhat, GS; Entrainment in Laboratory Simulations of Cumulus Cloud Flows. **American Geophysical Union, abstract #A21D-0127,** Fall Meeting, December 2010.

Srikanth, T; Dixit, Harish N; & Govindarajan, Rama; Shedding behaviour in low past an inline oscillating square cylinder. **Proceedings of IUTAM Symposium on Bluff Body Wakes, 2010.**

Narasimha, R; Diwan, Sourabh S; Subrahmanyam, Duvvuri; Sreenivas, KR; and Bhat, GS; Laboratory simulations of cumulus cloud flows explain the entrainment anomaly, **American Physical Society-Division of Fluid Dynamics, 63rd Annual Meeting (DFD10),** Long Beach, California, 21-23 November 2010.

Suryanarayanan, S; Narasimha, R; Is the growth rate of a turbulent mixing layer universal? **Bulletin of the American Physical Society, 2010.**

Book Chapters

Narasimha, R; A Fabulous Rationality: Poetry, Reason and Action in the Yoga-Vasistha. **In: Christopher Chapple (ed.), Yoga-Vasistha, US, 2012.**

Narasimha, R; The Yukti of Classical Indian Astronomical Science. **In: B.V. Sreekantan (ed). Foundations of Science (PHISPC). Centre for Studies in Civilizations,** New Delhi 2012.

Narasimha, R; Rockets in Mysore and Britain (AD 1750-1850). In: Harbans Mukhia (ed). **History of Technology in India, Vol. II, Indian National Science Academy pp. 804-822,** 2012.

Narasimha, R; Pramanas, proofs and the yukti of classical Indic Science. **In: Arun Bala (ed). Asia-Europe Dialogue and the Making of Modern Science, Palgrave Macmillan, 2012.** (in press)

Narasimha, R; Satish Dhawan. In: P Davidson et al (ed.). **A Voyage through Turbulence, Cambridge University Press. 2011.**

Narasimha, R; Culture views Nature: Bacon and Samkhya compared. **In: R Narasimha & S. Menon (eds). Nature and Culture (PHIPSC, Vol.14 pt.1), Centre for Studies in Civilizations,** New Delhi, 2011.

Roy, Anubhab; & Govindarajan, Rama; An introduction to hydrodynamic stability. **In: J Murali Krishnan (ed.). Rheology of Complex Fluids, Springer, 2010.**

Book
Narasimha, R; & Menon, S; (eds), **Nature and Culture (PHIPSC, Vol.14 pt.1), Centre for Studies in Civilizations,** New Delhi, 2011.

EVOLUTIONARY AND ORGANISMAL BIOLOGY UNIT

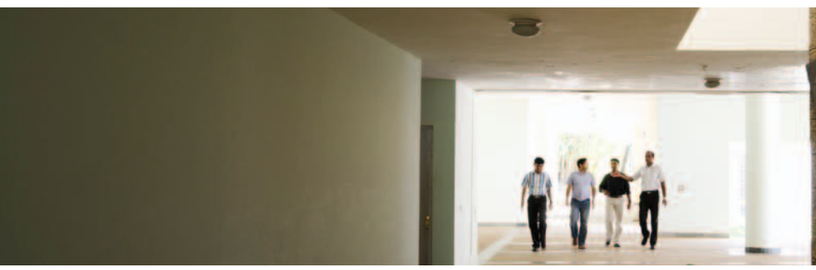
Kannan, NN; Reveendran, R; Hari Dass, S; Manjunatha, T; and Sharma, VK; Temperature can entrain egg laying rhythm of *Drosophila* but may not be a stronger zeitgeber than light. **Journal of Insect Physiology 58,** 245-255 (2012).

Lone, SR; Chakraverthi, A; and Sharma, VK; Sex and age related changes in the locomotor activity and phototactic behaviors of two closely related species of *Camponotus* ants. **Journal of Insect Physiology 58,** 75-82 (2012).

Lone, SR; Ilangovan, VM; Murugan and Sharma, VK; Short- and long-day responses in the pre-adult developmental duration of two species of *Camponotus* ants. **Chronobiology International 28,** 163-169 (2011).

Lone, SR; Sadanandappa, MK; and Sharma, VK; Cyclic presence and absence of conspecifics alters circadian clock phase but does not entrain the locomotor activity rhythm of the fruit fly *Drosophila melanogaster.* **Chronobiology International 28,** 497-508 (2011).

Lone, SR; and Sharma, VK; Circadian consequence of socio-sexual interactions in fruit flies *Drosophila melanogaster.* **PLoS One 6 e28336** (2011).



Lone, SR; and Sharma, VK; Timekeeping through social contacts: social synchronization of circadian locomotor activity rhythm in the carpenter ant *Camponotus paria.* **Chronobiology International 28,** 862-872 (2011).

Lone, SR; and Sharma, VK; Social synchronization of circadian locomotor activity rhythm in the fruit fly *Drosophila melanogaster.* **Journal of Experimental Biology 214,** 3742-3750 (2011).

Sivaperumal, R; Subramanian, P; Yadav, P; and Sharma, VK; Analysis of circadian locomotor rhythms in *vg* and *cry*^{b} mutants of *Drosophila melanogaster* under different light-dark regimes. **Biological Rhythm Research 42,** 321-335 (2011).

Sivaperumal, R; Subramanian, P; Yadav, P; and Sharma, VK; Analysis of light pulse induced phase shift in locomotor activity rhythm of *vg* and *Cry*^{b} mutants of *Drosophila melanogaster.* **Journal of Pharmaceutical Science and Research 2:433-444** (2010).

Shetty, N; and Vidya, TNC; To split or not to split: the case of the African elephant. **Current Science, 100,** 810-812 (2011).

Lone, SR; Ilangovan, V; Murugan, M; and Sharma, VK; Circadian resonance in the development of two sympatric species of *Camponotus* ants. **Journal of Insect Physiology 56:**1611-1616 (2010).

Vidya, TNC; and Thuppil, V; Immediate behavioural responses of humans and Asian elephants in the context of road traffic in southern India. **Biological Conservation, 143,** 1891-1900 (2010).

Sheeba, V; Fogle, KJ; and Holmes, TC; Persistence of morning anticipation behavior and high amplitude morning startle response following functional loss of small ventral lateral neurons in *Drosophila.* **PLoS One 5,** e11628 (2010).

Dey, S; Bose, J; and Joshi, AJ; Adaptation to larval crowding in *Drosophila ananassae* leads to the evolution of population stability. **Ecology and Evolution, 2(5),** 941-951, (2012)

INTERNATIONAL CENTRE FOR MATERIALS SCIENCES

CNR, Rao; HSSR, Matte; KS, Subrahmanyam; and U, Maitra; Unusual magnetic properties of graphene and related materials, **Chemical Science 3,** 45, 2012.

P, Kumar; B, Das; B, Chitara; KS, Subrahmanyam; K, Gopalakrishnan; SB, Krupanidhi; and CNR, Rao; Novel radiation induced properties of graphene and related materials, **Macromolecular Chemistry and Physics (Perspective) 213,** 1146 (2012).

CNR, Rao; U, Maitra; KS, Subrahmanyam; K, Gopalakrishnan; N, Kumar; R, Kumar; and A, Govindaraj; Potential of nanocarbons and related substances as adsorbents and chemical storage materials for H_2, CO_2 and other gases, **Indian Journal of Chemistry (50th Anniversary Issue),** 51A, 15 (2012).

CNR, Rao; A, Sundaresan; and R, Saha; Multiferroic and magnetoelectric oxides: The emerging scenario, **Journal of Physical Chemistry Letters (Perspective) 3,** 2237 (2012).

Loukya, B; Zhang, X; Gupta, A; and Ranjan, Datta; Electron magnetic chiral dichroism in CrO_2 thin films using monochromatic probe illumination in a transmission electron microscope. **Journal of Magnetism and Magnetic Materials, 324,** 3754 - 3761 (2012).

Ranjan Datta; Loukya, B; Li, N; and Gupta, A; Structural features of epitaxial $NiFe_2O_4$ thin films grown on different substrates by direct liquid injection chemical vapor deposition. **Journal of Crystal Growth, 345,** 44 - 50 (2012).

Sanyal, U; Ranjan Datta and Jagirdar, B; Colloidal calcium nanoparticles: digestive ripening in presence of a capping agent and coalescence of particles under an electron beam. **RSC Advances, 2,** 259 - 263 (2012).

Meng, FY; McFelea, H; Ranjan Datta, Chowdhury, U; Werkhoven, C; Arena, C; and Mahajan, S; Origin of predominantly a type dislocations in InGaN layers and wells grown on (0001) GaN. **Journal of Applied Physics, 110,** 073503 (2011).

DJ, Late; U, Maitra; LS, Panchakarla; UV, Waghmare; and CNR, Rao; Temperature effects on the Raman spectra of graphenes: Dependence on the number of layers and doping, **Journal of Physics: Condensed Matter 23,** 055303 (2011).

KS, Subrahmanyam; P, Kumar; U, Maitra; A, Govindaraj; KPSS, Hembaram; UV, Waghmare; and CNR, Rao; Chemical storage of hydrogen in few-layer graphene, **Proceedings of National Academy of Sciences (PNAS) 108,** 2674 (2011).

R, Saha; A, Shireen; AK, Bera; SN, Shirodkar; Y, Sundarayya; N, Kalarikkal; SM, Yusuf; UV, Waghmare; A, Sundaresan; and CNR, Rao; Structure and magnetic properties of the $Al_{1-x}Ga_xFeO_3$ family of oxides: A combined experimental and theoretical study, **Journal of Solid State Chemistry 184,** 494 (2011).

A, Shireen; R, Saha; A, Sundaresan; and CNR, Rao; Multiferroic and magnetodielectric properties of the $Al_{1-x}Ga_xFeO_3$ family of oxides, **Journal of Materials Chemistry (Commun.) 21,** 57 (2011).

P, Kumar; LS, Panchakarla; and CNR, Rao; Laser-induced unzipping of carbon nanotubes to yield graphene nanoribbons, **Nanoscale 3,** 2127 (2011).

U, Maitra; B, Das; N, Kumar; A, Sundaresan; and CNR, Rao; Ferromagnetism exhibited by nanoparticles of noble metals, **ChemPhysChem 12,** 2322 (2011).

K, Moses; LS, Panchakarla; HSSR, Matte; B, Govindarao; and CNR, Rao; Synthesis, characterization and spectroscopy of composites of graphene with CdSe and CdS nanoparticles, **Indian Journal of Chemistry (P.C. Ray Issue) 50A,** 1239 2011.

N, Kumar; KS, Subrahmanyam; P, Chaturvedy; K, Raidongia; A, Govindaraj; KPSS, Hembram; AK, Misra; U, Waghmare; and CNR, Rao; Remarkable uptake of CO_2 and CH_4 by graphene-like borocarbonitrides, BxCyNz, **ChemSusChem 4,** 1662 (2011).

CNR, Rao; KS, Subrahmanyam; HSSR, Matte; U, Maitra; K, Moses; and A, Govindaraj; Graphene: Synthesis, functionalization and properties, **International Journal of Modern Physics 30,** 4107 (2011).

Ramakrishna, Matte HSS; Blake, Plowman; Ranjan, Datta; and Rao, CNR; Graphene analogues of layered metal selenides. **Dalton Transactions, 40,** 10322 - 10325 (2011).

Loukya, B; Sowjanya, PK; Dileep, Shipra, R; Kanuri, S; Panchakarla, LS; and Ranjan Datta, Controlling structural quality of ZnO thin film on c-plane sapphire during pulsed laser deposition. **Journal of Crystal Growth, 329,** 20 - 26 (2011).

Datta, KKR; Jagadeesan, D; Kulkarni, C; Kamath, A; Ranjan Datta and Eswaramoorthy, M; Observation of Pore-switching Behaviour in Porous Layered Carbon through Mesoscale Order-Disorder Transformation. **Angew. Chem. Int. Ed, 50,** 3929 - 3933 (2011).

Dileep, K; Panchakarla, LS; Balasubramanian, K; Waghmare, UV; and Ranjan Datta, Electron energy loss spectroscopy of ZnO nanocrystals with different oxygen vacancy concentrations. **Journal of Applied Physics, 109,** 063523 (2011).

CNR, Rao; AK, Sood; R, Voggu; and KS, Subrahmanyam; Some novel attributes of graphene, **Journal of Physical Chemistry Letters (Perspective) 1,** 572 (2010).

LS, Panchakarla; Y, Sundarayya; S, Manjunatha; A, Sundaresan; and CNR, Rao; On the defect origin of room-temperature magnetism-exhibited by metal oxide nanoparticles, **ChemPhysChem 11,** 1673 (2010).

UA, Palnitkar; RV, Kashid; MA, Mose; DS, Joag; LS, Panchakarla; and CNR, Rao; Remarkably low turn-on field emission in undoped, nitrogen-doped and boron-doped graphene, **Applied Physics Letters 97,** 063102 (2010).

P, Kumar; LS, Panchakarla; SV, Bhat; U, Maitra; KS, Subrahmanyam; and CNR, Rao; Photoluminescence, white-light emitting properties and related aspects of ZnO nanoparticles admixed with graphene and GaN, **Nanotechnology 21,** 385701 (2010).

K, Raidongia; A, Gomati; and CNR, Rao; Synthesis and characterization of nanoparticles, nanotubes, nanopans and graphene-like structure of BN, **Israel Journal of Chemistry (Special Nano Number) 50,** 399 (2010).

Raidongia, K; Nag, A; Ranjan Datta and Rao, CNR; Nanopans and nanosheets formed by graphene-like BN. **Nanoscale (RSC),** (2010).

Venu, K; Kanuri, S; Raidongia, K; Hembram, KPSS; Waghmare, UV; and Ranjan Datta, Band gap and chemically ordered domain structure of a graphene analogue BxCyNz. **Solid State Commun, 150,** 2262 - 2265 (2010).

Radha, B; Arif, M; Ranjan Datta, Kundu, T; Kulkarni, GU; Movable Au microplates as fluorescence enhancing substrates for live cells. **Nano Research, 3,** 738 - 747 (2010).

Ranjan Datta, Kanuri, S; Karthik, SV; Mazumdar, D; Ma, JX; and Gupta, A; Formation of anti-phase domains in $NiFe_2O_4$ thin films deposited on different substrates. **Appl. Phys. Lett, 97,** 7, 071907 (2010).

Indrani Sen, Gopinath, K; Ranjan Datta, Ramamurty Upadrasta, Fatigue in Ti-6Al-4V-B alloys. **Acta Materialia, 58,** 6799 - 6809 (2010).

Ramakrishna Matte, HSS; Gomathi, A; Manna, Arun K; Dattatray J Late; Ranjan Datta; Pati, Swapan K; and Rao, CNR; Graphene analogues of MoS_2 and WS_2. **Angew. Chem. Int. Ed, 49,** 4059 - 4062 (2010).

Nag, Angshuman; Raidongia, Kalyan; Hembram, Kailash PSS; Datta, Ranjan; Waghmare, Umesh V; and Rao, CNR; Graphene Analogues of BN: Novel Synthesis and Properties. **ACS Nano, 3,** 1539 - 1544 (2010).

Raidongia, Kalyan; Nag, Angshuman; Hembram, KPSS; Waghmare, Umesh V; Datta, Ranjan; and Rao, CNR; BCN: A Graphene Analogue with Remarkable Adsorptive Properties. **Chemistry - A European Journal, 16,** 149 - 157 (2010).

Kumar, P; Kumar, M; Shivaprasad, SM; (7x7) reconstruction as barrier for Schottky-barrier formation at the Ga/Si(111) interface. **Applied Physics Letters, 97,** 122105, 2010.

Kumar, P; Jithesh, K; Shivaprasad, SM; Ga induced superstructures as templates for lattice matched hetroepitaxial growth of GaN on Si(111) substrate. **Applied Physics Letters, 97,** 221913, 2010.

Jithesh, K; Govind, Kumar, M; Shivaprasad, SM; Clustering and layering of In adatoms on low and high index silicon surfaces: A comparative study. **Surface Science, 604,** 1972, 2010.

Nie, Y; Wang, Y; Pan, JS; Mehta, BR; Khanuja, M; Shivaprasad, SM; Sun, CQ; CuPd interface charge and energy quantum entrapment: A tight-binding and XPS investigation. **Applied Surface Science, 257,** 727, 2010.

Sun, CQ; Nie, WY; Guang, Y; Mehta, BR; Shivaprasad, SM; Sun, Y; pan, Lk; Zhua, S; Interface quantum trap depression and charge polarization in the CuPd and AgPd bimetallic alloy catalysts. **Physical Chemistry Chemical Physics, 12,** 3121, 2010

Chauhan, AKS; Govind, JK; Shivaprasad, SM; Adsorption/desorption kinetics of Na atoms on reconstructed Si (111)-7 x 7 surface. **Thin Solid Films 519,** 1012, 2010.

Sharma, H; Sharma, SN; Singh, S; Mehra, NC; Singh, G; Shivaprasad, SM; Comparison of the properties of composition-tunable CdSe–ZnSe and $Zn_xCd_{1-x}Se$ nanocrystallites: Single- and double-pot synthesis approach. **Materials Chemistry and Physics, 124,** 670, 2010.

Bhattacharya, S; Shivaprasad, SM; Gajbhiye, NS; Variation of magnetic ordering in ε-Fe_3N nanoparticles. **Chemical Physics Letters, 496,** 122, 2010.

Sharma, SN; Sharma, H; Singh, S; Mehra, RM; Singh, G; Shivaprasad, SM; Single pot synthesis of composition tunable CdSe-ZnSe (core-shell) and $Zn_xCd_{1-x}Se$ (ternary alloy) nanocrystals with high luminescence and stability. **Materials Research Innovations, 14,** 62, 2010.

Bhattacharya, S; Kurian, S; Shivaprasad, SM; Gajbhiye, NS; Synthesis and magnetic characterization of $CoMoN_2$ nanoparticles. **Journal of Nanoparticle Research, 12,** 1107, 2010.

Kumar, P; Kumar, M; Mehta, BR; Shivaprasad, SM; Ga-induced restructuring of Si(5 5 12) – 2 × 1 reconstructed surface at room temperature. **Surface Science, 605,** 1426, 2011.

Kuyyalli, J; Tangi, M; Shivaprasad, SM; Dependence of crystal orientation and bandgap on substrate temperature of molecular-beam epitaxy grown InN on bare Al_2O_3 (0001). **Journal Applied Physics, 109,** 093513, 2011.

Kumar, P; Kumar, M; Govind; Mehta, BR; Shivaprasad, SM; Adsorption kinetics of low-dimensional Ga structures on Si(5 5 12)-2x1 trenched templates. **International Journal of Nanoscience, 1,** 117, 2011.

Kesaria, M; Shetty, S; Shivaprasad, SM; Spontaneous formation of GaN nanostructures by molecular beam epitaxy. **Journal of Crystal Growth, 326,** 191, 2011.

Galkin, KN; Kumar, M; Shivaprasad, SM; Galkin, NG; The model of the magnesium silicide phase (2/3√3×2/3√3)-R30° on Si(111). **Physics Procedia, 11,** 47, 2011.

Galkin, KN; Kumar, M; Shivaprasad, SM; Galkin, NG AES and EELS study of desorption of magnesium silicide films on Si(111). **Physics Procedia, 11,** 51, 2011.

Kesaria, M; Shetty, S; Shivaprasad, SM; Transformation of c-oriented nanowall network to a flat morphology in GaN films on c-plane sapphire. **Materials Research Bulletin, 46,**1811, 2011.

Kesaria, M; Shetty, S; Shivaprasad, SM; Evidence for Dislocation Induced Spontaneous Formation of GaN Nanowalls and Nanocolumns on bare C-Plane Sapphire. **Crystal Growth and Design, 11,** 4900, 2011.

Kesaria, M; Shivaprasad, SM; Nitrogen flux induced GaN nanostructure nucleation at misfit dislocations on Al2O3(0001). **Applied Physics Letters, 99,** 143105, 2011.

Kumar, P; Kuyyalli, J; Kumar, M; Shivaprasad, SM; A superstructural 2D-phase diagram for Ga on the Si(111)-7x7 system. **Solid State Communications, 151,** 1758, 2011.

Mitra, J; Abraham, GJ; Kesaria, M; Bhal, S; Gupta, A; Sivaprasad, SM; Viswanadham, CS; Kulkarni, UD; Dey, GK; Role of substrate temperature in the pulsed laser deposition of zirconium oxide thin film. **Materials Science Forum, 710,** 757, 2012.

Kumar, P; Kumar, M; Sivaprasad, SM; Ga induced 2D superstructural phase diagram on trenched Si(5 5 12) surface. **Surface Science, 606,** 1045, 2012.

Kumar, P; Tangi, M; Kesaria, M; Shetty, S; Shivaprasad, SM; Growth of aligned wurtzite GaN nanorods on Si(111): Role of Silicon nitride intermediate layer. **MRS proceeding, (2012) 1411,** mrsf11-1411-ee09-24.

Kulriya, PK; Mehta, BR; Agarwal, DC; Kumar, P; Shivaprasad, SM; Giant enhancement in ferromagnetic properties of Pd nanoparticles induced by intentionally created defects. **Journal of Applied Physics, 112,** 014318, 3012.

Viswanatha, Ranjani; Doron, Naveh; James, R Chelikowsky; Leeor, Kronik; and Sarma, DD; Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. **J. Phys. Chem. Lett., (2012).** In Press.

Sergio, Brovelli; Christophe, Galland; Viswanatha, Ranjani; and Klimov, Victor I; Tuning Radiative Recombination in Cu-doped Nanocrystals via Electrochemical Control of Surface Trapping. **NanoLetters, (2012).** In Press.

K, Hima Nagamanasa; Gokhale, Shreyas; Ganapathy, Rajesh; and Sood, AK; Confined Glassy Dynamics at Grain Boundaries in Colloidal Crystals. **Proceeding of the National Academy of Sciences (U.S.A.) 108,** 11323 (2011).

MOLECULAR BIOLOGY AND GENETICS UNIT

Selvi, RB; Krishna, DV; Ostwal, YB; and Kundu, TK; Modulators of Chromatin modifying enzymes in transcription and disease – A Connotation to Epigenetic Therapy. **Biochim Biophys Acta 1799,** 810 - 828 (2010).

Selvi, RB; Cassel, JC; Kundu, TK; and Boutillier, AL; Tuning acetylation levels with HAT activators: therapeutic strategy in neurodegenerative diseases. **Biochim Biophys Acta 1799,** 840 - 853 (2010).

Arif, M; Shandilya, J; Senapati, P; and Kundu, TK; Protein lysine acetylation in cellular function and its role in cancer manifestation, **Biochim Biophys Acta 1799,** 702 - 716 (2010).

Arif, M; Selvi, BR; and Kundu, TK; Lysine acetylation: the tale of a modification from transcription regulation to metabolism. **Chembiochem 11,** 1501 - 4 (2010).

Arif, M; Vedamurthy, BM; Choudhari, R; Ostwal, YB; Mantelingu, K; Kodaganur, GS; and Kundu, TK; Nitric oxide-mediated histone hyperacetylation in oral cancer: target for a water-soluble HAT inhibitor, CTK7A. **Chemistry and Biology 17,** 903 - 913 (2010).

Ramana, LN; Sethuraman, S; Ranga, U; and Krishnan, UM; Development of a liposomal nanodelivery system for nevirapine. **J Biomed Sci 17 - 57** (2010).

Madhavi, Y; Puliyel, JM; Mathew, JL; Raghuram, N; Phadke, A; Shiva, M; Srinivasan, S; Paul, Y; Srivastava, RN; Parthasarathy, A; Gupta, S; Ranga, U; Lakshmi, VV; Joshi, N; Nath, I; Gulhati, CM; Chatterjee, P; Jain, A; Priya, R; Dasgupta, R; Sridhar, S; Dabade, G; Gopakumar, KM; Abrol, D; Santhosh, MR; Srivastava, S; Visalakshi, S; Bhargava, A; Sarojini, NB; Sehgal, D; Selvaraj, S; Banerji, D; and, Evidence-based National Vaccine Policy. **Indian J Med Res.131,** 617 - 628 (2010).

Kumar, GG; Mahadevan, A; Guruprasad, AS; Jerry, ME; Kovoor, MD; P, Satishchandra; Nath, A; Udaykumar, Ranga; and Shankar, SK; Eccentric target sign in cerebral toxoplasmosis: neuropathological correlate to the imaging feature, **J Magn Reson Imaging. 31,** 1469 - 1472 (2010).

Sanchari, Bhattacharyya; Roshan, Elizabeth Rajan; Yalla, Swarupa; Ujjwal, Rathore; Anjali, Verma; Udaykumar, Ranga; and Raghavan, Varadarajan; Design of a non-glycosylated outer domain derived HIV-1 gp120 immunogen that binds to CD4 and induces neutralizing antibodies. **Journal of Biological Chemistry 285,** 27100 - 27110 (2010).

Jayashree, Ladha; Sainitin, Donakonda; Shipra, Agrawal; Balaram, Thota; MR, Srividya; S, Sridevi; A, Arivazhagan; K, Thennarasu; Anandh, Balasubramaniam; BA, Chandramouli; AS, Hegde; Paturu, Kondaiah; Kumaravel, Somasundaram; Vani, Santosh; and Satyanarayana, MR Rao; Glioblastoma specific protein interaction network identifies PP1A and CSK21 as connecting molecules between cell cycle associated genes. **Cancer Research 70,** 6437 - 6447 (2010).

Ratnapriya, R; J, Vijai; J, Kadandale; R, Iyer; K, Radhakrishnan; and A, Anand; A locus for juvenile myoclonic epilepsy maps to 2q33-q36, Human Genetics (2010).

Santosh, V; Arivazhagan, A; Sreekantha Reddy, P; Srinivasan,H; Thota, B; Srividya, MR; Vrinda, M; Sridevi, S; Shailaja, BC; Samuel, C; Prasanna, KV; Thennarasu, K; Balasubramaniam, A; Chandramouli, BA; Hegde, .AS; Somasundaram, K; Kondaiah, P; and Rao, MRS; Grade specific expression of IGFBP-2, -3 and -5 in astrocytomas: IGFBP3 emerges as a strong predictor of survival in patients with newly diagnosed glioblastoma. **Cancer Epidemiology, Biomarkers and Prevention 19,** 1399 - 1408 (2010).

Sreekanthreddy, P; Srinivasan, Harish; Mohan Kumar, Durairaj; Nijaguna, Mamatha; S, Sridevi; M, Vrinda; A, Arivazhagan; Anandh, Balasubramaniam; Hegde, AS; Chandramouli, A; Santosh, Vani; Rao, MRS; Kondaiah, Puturu; and Somasundaram, umaravel; Identification of potential serum biomarkers of glioblastoma: Serum osteopontin levels correlate with poor prognosis. **Cancer Epidemiology, Biomarkers and Prevention 19,** 1409 – 1422 (2010).

Ranga, Udaykumar; Banerjea, Akhil; Chakrabarti, Sekhar; Mitra, Debashish; HIV/AIDS research in India-Past, Present and future. **Current Science 98,** 335 - 345 (2010).

Ranga, Udaykumar; The Saga of the HIV Controversy: Nobel Prize in Physiology or Medicine – 2008. **Resonance 14 ,** 472 - 498 (2010).

Sreenath, K; Pavithra, L; Singh, S; Sinha, S; Dash, PK; Siddappa, NB; Ranga, U; Mitra, D; Chattopadhyay, S; Nuclear Matrix protein SMAR1 represses HIV-1 LTR mediated transcription through chromatin remodeling. **Virology 400,** 76 - 85 (2010).

Karthigeyan, D; Prasad, SB; Shandilya, J; Agrawal, S; and Kundu, TK; Biology of Aurora A kinase: Implications in cancer manifestation and therapy. **Med Res Rev (2010).**

Das, C; Gadad, SS; and Kundu, TK; Human Positive Coactivator 4 Controls Heterochromatinization and Silencing of Neural Gene Expression by Interacting with REST/NRSF and CoREST. **J Mol Biol 397,** 1 - 12 (2010).

Gadad, SS; Shandilya, J; Kishore, AH; and Kundu, TK; NPM3, a member of the nucleophosmin/nucleoplasmin family, enhances activator-dependent transcription. **Biochemistry 49,** 1355 - 1357 (2010).

Selvi, BR; Batta, K; Kishore, AH; Mantelingu, K; Varier, RA; Balasubramanyam, K; Pradhan, SK; Dasgupta, D; Sriram, S; Agrawal, S; and Kundu,TK; Identification of a Novel Inhibitor of Coactivator-associated Arginine Methyltransferase 1 (CARM1)-mediated Methylation of Histone H3 Arg-17. **J Biol Chem 285,** 7143 - 7152 (2010).

Venu, P; Chakraborty, S; and Inamdar, M; Analysis of long- term culture properties and pluripotent character of two sibling human embryonic stem cell lines derived from discarded embryos. **In vitro Cellular & Developmental Biology - Animal 46,** 200 - 205 (2010).

Radha, B; Arif, M; Datta, R; Kundu, TK; Kulkarni, GU; (2010). Movable Au microplates as fluorescence enhancing substrates for live cells. **Nano Research, 3,** 738 - 747

Dehnugara, Tushna; Dhar, Surbhi; and Rao, MRS; An In Vitro, Short-Term Culture Method for Mammalian Haploid Round Spermatids Amenable for Molecular Manipulation. **Molecular Reproduction and Development (2011)**

Laha, Suparna; Das, Shankar P; Hajra, Sujata; Sanyal, Kaustuv; and Sinha, Pratima; Functional characterization of the Saccharomyces cerevisiae protein Chl1 reveals the role of sister chromatid cohesion in the maintenance of spindle length during S-phase arrest. **BMC Genetics 12,** 83 (2011).

Roy, Babhrubahan; and Sanyal, Kaustuv; Diversity in Requirement of Genetic and Epigenetic Factors for Centromere Function in Fungi. **Eukaryotic Cell 10,** 1384 - 1395 (2011).

Bulusu, Vinay; Jayaraman, Vijay; and Balaram, Hemalatha; Metabolic Fate of Fumarate, a Side Product of the Purine Salvage Pathway in the Intraerythrocytic Stages of Plasmodium falciparum. **J Biol Chem 286,** 9236 - 9245 (2011).

Thakur, Jitendra; and Sanyal, Kaustuv; The essentiality of the fungus specific Dam1complex is correlated with one kinetochore one microtubule interaction present throughout the cell cycle, independent of the nature of a centromere. **Eukaryotic Cell 10,** 1295 - 1305 (2011).

Roy, Babhrubahan; Burrack, Laura S; Lone, Museer A; Berman, Judith; and Sanyal, Kaustuv; CaMtw1, a member of the evolutionarily conserved Mis12 kinetochore protein family, is required for efficient inner kinetochore assembly in the pathogenic yeast *Candida albicans,* **Molecular Microbiology 80,** 14 - 32 (2011).

SS, Gadad; P, Senapati; Syed, SH; Rajan, RE; Shandilya, J; Swaminathan, V; Chatterjee, S; Colombo, E; Dimitrov, S; Pelicci, PG; Ranga, U; Kundu, TK; (2011). The multifunctional protein nucleophosmin (NPM1) is a human linker histone H1 chaperone. **Biochemistry 50 (14):** 2780-9.

Debnath, S; Chatterjee, S; Arif, M; Kundu, TK; Roy, S; (2011). Peptide-protein interactions suggest that acetylation of lysines 381 and 382 of p53 is important for positive coactivator 4-p53 interaction. **J Biol Chem 286 (28):**25076-87

SS, Gadad; Rajan, RE; Senapati, P; Chatterjee, S; Shandilya, J; Dash, PK; Ranga, U; Kundu, TK; (2011) HIV-1 infection induces acetylation of NPM1 that facilitates Tat localization and enhances viral transactivation. **J Mol Biol 410 (5):** 997-1007.

Maity, D; Manna, AK; Karthigeyan, D; Kundu, TK; Pati, SK; Govindaraju, T; (2011). Visible- near-infrared and fluorescent copper sensors based on julolidine conjugates: selective detection and fluorescence imaging in living cells. **Chemistry 17 (40):** 11152-61

KS, Vimaleswaran; V, Radha; S, Ghosh; Partha, P Majumder; Rao, MRS; and V, Mohan; Uncoupling Protein 2 and 3 Gene Polymorphisms and Their Association with Type 2 Diabetes in Asian Indians. **Diabetes Technology & Therapeutics (2011)** 13(1): 19-25.

Bodhini, D; Radha, V; Ghosh, S; Sanapala, KR; Majumder, PP; Rao, MR; Mohan, V; **Association of Calpain 10 gene polymorphism with Type 2 Diabetes mellitus in Southern Indians Metabolism.** (2011) 60(5):681-688.

Bodhini, D; Radha, V; Ghosh, S; Majumder, PP; Rao, MR; Mohan, V; **Glut 4 Gene polymorphisms and their association with Type 2 Diabetes in South Asians Diabetes Technol Ther.** (2011) 13, 913-920.

Screening ethnically diverse human embryonic stem cells identifies a chromosome 20 minimal amplicon conferring growth advantage. **Nature Biotechnology doi:10.1038/nbt.2051** (Nov 2011).

Kulkarni, V; Khadilkar, R; Srivathsa, MS; and Inamdar, MS; Asrij Maintains the Stem Cell Niche and controls differentiation during Drosophila Lymph Gland Hematopoiesis. **PLoSOne, 6(11)** 2011.

Inamdar, MS; Healy, L; Sinha, A; Stacey, G; Global Solutions to the Challenges of Setting up and Managing a Stem Cell Laboratory. **Stem Cell Reviews and Reports DOI: 10.1007/s12015-011-9326-7** (Oct 2011).

Shetty, R; and Inamdar, MS; Derivation of human embryonic stem cell lines from poor quality embryos. **Methods Mol Biol.**

Bachu, M; Anilbabu, M; Rajesh, MV; Narayanaiah, C; Mahadevan, A; Shankar, SK; Satish, KS; Kundu, TK; Ranga, U; (2012) Sequence insertions in the HIV-1 subtype C viral promoter predominantly generate an additional NF-κB binding site. **AIDS Res Hum Retroviruses.**

Modak, R; Das Mitra, S; Krishnamoorthy, P; Bhat, A; Banerjee, A; Gowsica, BR; Bhuvana, M; Dhanikachalam, V; Natesan, K; Shome, R; Shome, BR; Kundu, TK; (2012) Histone H3K14 and H4K8 hyperacetylation is associated with Escherichia coli induced mastitis in mice. **Epigenetics 7(5)**

Arivazhagan, A; Durairaj, MK; Vinay, S; Sridevi, S; Thota, B; Srividya, MR; Irene, RP; Prasanna, K; Thennarasu, K Mondal N; Hegde, AS; Chandramouli, BA; Santosh, V; Rao, MRS; Kondaiah, P; and Somasundaram, K; Higher

TOP2A levels predict better prognosis in GBM patiens receiving Temozolamide chemotherapy: Identification of temozolamide as a Topo 2A inhibitor. **Journal of Neuro-oncology (2012) 107,** 289-297

Dhar, S; Thota, A; and Rao, MRS; Insights into the role of Bromodomain testis- specific(Brdt) in acetylated histone H4 dependent chromatin remodeling in mammalian spermiogenesis. **J. Biol. Chem. 2012** (2012) 287, 6387-6405

Thakur, Jitendra; and Sanyal, Kaustuv; (2012) A coordinated interdependent protein Circuitry stabilizes the kinetochore ensemble to protect CENP-A in the human pathogenic Yeast Candida albicans. **PLoS Genetics 8:** e1002661

Sanyal, Kaustuv; (2012) How do microbial pathogens make CENs? **PLoS Pathogens 8,** e1002463.

Sudhir, H Ranganath; Oren, Levy; Maneesha, S Inamdar; and Jeffrey, Karp; Harnessing the Mesenchymal Stem Cell Secretome for the Treatment of Cardiovascular Disease. **Cell Stem Cell 10,** 244-258 (2012), doi:10.1016/j.stem.2012.02.005.

Mamta, Jain; Ganesh, P Bhat; VijayRaghavan, K; and Inamdar, M S; Rudhira/BCAS3 is a cytoskeletal protein that controls Cdc42 activation and directional cell migration during angiogenesis. **Exp. Cell. Res., 318 (6)** doi:10.1016/j.yexcr.2012.01.016. (2012).

NEW CHEMISTRY UNIT

Amareshwar, V; Mishra, NC; Ila, H; 2-Phenyl-4-bis(methylthio)methyleneoxazol-5-one: versatile template for diversity oriented synthesis of heterocycles. **Organic & Biomolecular Chemistry 2011,** 9, (16), 5793-5801.

Avinash, MB; Govindaraju, T; Engineering Molecular Organization of Naphthalenediimides: Large Nanosheets with Metallic Conductivity and Attoliter Containers. **Advanced Functional Materials 2011,** 21, (20), 3875-3882.

Avinash, MB; Govindaraju, T; A bio-inspired design strategy: Organization of tryptophan-appended naphthalenediimide into well-defined architectures induced by molecular interactions. **Nanoscale 2011,** 3, (6), 2536-2543.

Basheer, EA; Parida, P; Pati, SK; Electronic and magnetic properties of BNC nanoribbons: a detailed computational study. **New Journal of Physics 2011,** 13.

Bhat, SV; Govindaraj, A; Rao, CNR; Hybrid solar cell based on P3HT-ZnO nanoparticle blend in the inverted device configuration. **Solar Energy Materials and Solar Cells 2011,** 95, (8), 2318-2321.

Brovelli, S; Schaller, RD; Crooker, SA; García-Santamaría, F; Chen, Y; Viswanatha, R; Hollingsworth, JA; Htoon, H; Klimov, VI, Nano-engineered electron–hole exchange interaction controls exciton dynamics in core–shell semiconductor nanocrystals. **Nature Communications 2011,** 2, 280.

Chakraborty, A; Gurunatha, KL; Muthulakshmi, A; Dutta, S; Pati, SK; Maji, TK, Assembly of trinuclear and tetranuclear building units of Cu2+ towards two 1D magnetic systems: synthesis and magneto-structural correlations. **Dalton Transactions 2012,** 41, (19), 5879-5888.

Chaturbedy, P; Matte, HSSR; Voggu, R; Govindaraj, A; Rao, CNR; Self-assembly of C-60, SWNTs and few-layer graphene and their binary composites at the organic-aqueous interface. **Journal of Colloid and Interface Science 2011, 360,** (1), 249-255.

Chitara, B; Krupanidhi, SB; Rao, CNR, Solution processed reduced graphene oxide ultraviolet detector. **Applied Physics Letters 2011,** 99, (11).

Chitara, B; Lal, N; Krupanidhi, SB; Rao, CNR, Electroluminescence from GaN-polymer heterojunction. **Journal of Luminescence 2011,** 131, (12), 2612-2615.

Chitara, B; Panchakarla, LS; Krupanidhi, SB; Rao, CNR; Infrared Photodetectors Based on Reduced Graphene Oxide and Graphene Nanoribbons. **Advanced Materials 2011,** 23, (45), 5419-+.

Chitara, B; Panchakarla, LS; Krupanidhi, SB; Rao, CNR, UV Photodetectors Based on ZnO Nanorods: Role of Defect-Concentration. **Japanese Journal of Applied Physics 2011,** 50, (10).

Choudhury, D; Mandal, P; Mathieu, R; Hazarika, A; Rajan, S; Sundaresan, A; Waghmare, UV; Knut, R; Karis, O; Nordblad, P; Sarma, DD; Near-Room-Temperature Colossal Magnetodielectricity and Multiglass Properties in Partially Disordered La_1NiMnO_1. **Physical Review Letters 2012,** 108, (12), 127201.

Choudhury, D; Mukherjee, S; Mandal, P; Sundaresan, A; Waghmare, UV; Bhattacharjee, S; Mathieu, R; Lazor, P; Eriksson, O; Sanyal, B; Nordblad, P; Sharma, A; Bhat, SV; Karis, O; Sarma, DD, Tuning of dielectric properties and magnetism of $SrTiO_3$ by site-specific doping of Mn. **Physical Review B 2011, 84,** (12).

Das, B; Choudhury, B; Gomathi, A; Manna, AK; Pati, SK; Rao, CNR, Interaction of Inorganic Nanoparticles with Graphene. **Chemphyschem 2011, 12,** (5), 937-943.

De Cat, I; Guo, Z; George, SJ; Meijer, EW; Schenning, APHJ; De Feyter, S; Induction of Chirality in an Achiral Monolayer at the Liquid/Solid Interface by a Supramolecular Chiral Auxiliary. **Journal of the American Chemical Society 2012, 134,** (6), 3171-3177.

Dey, R; Haldar, R; Maji, TK; Ghoshal, D, Three-Dimensional Robust Porous Coordination Polymer with Schiff Base Site on the Pore Wall: Synthesis, Single-Crystal-to-Single-Crystal Reversibility, and Selective CO_2 Adsorption. **Crystal Growth & Design 2011, 11,** (9), 3905-3911.

Dey, T; Khuntia, P; Mahajan, AV; Kumar, N; Sundaresan, A, 119Sn NMR probe of magnetic fluctuations in SnO_2 nanoparticles. **Europhysics Letters 2011, 96,** (6).

Disseler, SM; Svensson, JN; Peter, SC; Byers, CP; Baines, C; Amato, A; Giblin, SR; Carretta, P; Graf, MJ, Competing interactions and magnetic frustration in Yb_4LiGe_4. **Physical Review B 2011, 84,** (17).

Eggeman, AS; Sundaresan, A; Rao, CNR; Midgley, PA; The structure of two new non-centrosymmetric phases of oxygen deficient bismuth manganite. **Journal of Materials Chemistry 2011, 21,** (39), 15417-15421.

Garcia-Santamaria, F; Brovelli, S; Viswanatha, R; Hollingsworth, JA; Htoon, H; Crooker, SA; Klimov, VI; Breakdown of Volume Scaling in Auger Recombination in CdSe/CdS Heteronanocrystals: The Role of the Core-Shell Interface. **Nano Letters 2011, 11,** (2), 687-693.

George, SJ; Tomovic, Z; Schenning, APHJ; Meijer, EW, Insight into the chiral induction in supramolecular stacks through preferential chiral solvation. **Chemical Communications 2011, 47,** (12), 3451-3453.
Ghosh, D; Periyasamy, G; Pati, SK; Density functional theoretical investigation of the aromatic nature of BN substituted benzene and four ring polyaromatic hydrocarbons. **Physical Chemistry Chemical Physics 2011, 13,** (46), 20627-20636.

Ghosh, S; Yamijala, SRKCS; Pati, SK; Rao, CNR; The interaction of halogen molecules with SWNTs and graphene. **RSC Advances 2012, 2,** (3), 1181-1188.

Govindaraju, T; Spontaneous self-assembly of aromatic cyclic dipeptide into fibre bundles with high thermal stability and propensity for gelation. **Supramolecular Chemistry 2011, 23,** (11), 759-767.

Govindaraju, T; Pandeeswar, M; Jayaramulu, K; Jaipuria, G; Atreya, HS; Spontaneous self-assembly of designed cyclic dipeptide (Phg-Phg) into two-dimensional nano- and mesosheets. **Supramolecular Chemistry 2011, 23,** (7), 487-492.

Haag, B; Mosrin, M; Ila, H; Malakhov, V; Knochel, P, Regio- and Chemoselective Metalation of Arenes and Heteroarenes Using Hindered Metal Amide Bases. **Angewandte Chemie-International Edition 2011, 50,** (42), 9794-9824.

Haldar, R; Maji, TK, A two-fold interpenetrated flexible bi-pillared-layer framework of Fe(II) with interesting solvent adsorption property. **Journal of Chemical Sciences 2011, 123,** (6), 883-890.

Haldar, R; Maji, TK; Selective carbon dioxide uptake and crystal-to-crystal transformation: porous 3D framework to 1D chain triggered by conformational change of the spacer. **Crystengcomm 2012,** 14, (2), 684-690.

Haldar, R; Rao, KV; George, SJ; Maji, TK; Exciplex Formation and Energy Transfer in a Self-Assembled Metal-Organic Hybrid System. **Chemistry-a European Journal 2012, 18,** (19), 5848-5852.

Harmening, T; Eckert, H; Fehse, CM; Sebastian, CP; Poettgen, R; 45Sc Solid State NMR studies of the silicides ScTSi (T=Co, Ni, Cu, Ru, Rh, Pd, Ir, Pt). **Journal of Solid State Chemistry 2011, 184,** (12), 3303-3309.

Iyer, AK; Peter, SC; EuLiGe2 and YbLiGe2-A Divalent and an Intermediate-Valent Compound with CaLiSi2-Type Structures. **European Journal of Inorganic Chemistry 2012, (11),** 1790-1794.

Jain, A; Rao, KV; Goswami, A; George, SJ, Metal selective co-ordinative self-assembly of pi-donors. **Journal of Chemical Sciences 2011, 123,** (6), 773-781.

Jain, A; Rao, KV; Kulkarni, C; George, A; George, SJ; Fluorescent coronene monoimide gels via H-bonding induced frustrated dipolar assembly. **Chemical Communications 2012, 48,** (10), 1467-1469.

Jain, A; Rao, KV; Mogera, U; Sagade, AA; George, SJ; Dynamic Self-Assembly of Charge-Transfer Nanofibers of Tetrathiafulvalene Derivatives with F(4)TCNQ. **Chemistry-a European Journal 2011, 17,** (44), 12355-12361.

Kanoo, P; Haldar, R; Cyriac, ST; Maji, TK; Coordination driven axial chirality in a microporous solid assembled from an achiral linker via in situ C-N coupling. **Chemical Communications 2011, 47,** (39), 11038-11040.

Khan, TA; Kumar, S; Venkatesh, C; Ila, H; Regioselective rapid analog synthesis of 1,3-(or 1,5-)diphenyl-4-aryl/heteroaryl-5-(or 3-)(methylthio)pyrazoles via Suzuki cross-coupling. **Tetrahedron 2011, 67,** (16), 2961-2968.

Korevaar, PA; George, SJ; Markvoort, AJ; Smulders, MMJ; Hilbers, PAJ; Schenning, APHJ; De Greef, TFA; Meijer, EW, Pathway complexity in supramolecular polymerization. **Nature 2012, 481,** (7382), 492-U103.

Kulkarni, C; Reddy, SK; George, SJ; Balasubramanian, S, Cooperativity in the stacking of benzene-1,3,5-tricarboxamide: The role of dispersion. **Chemical Physics Letters 2011, 515,** (4-6), 226-230.

Kumar, M; George, SJ, Spectroscopic Probing of the Dynamic Self-Assembly of an Amphiphilic Naphthalene Diimide Exhibiting Reversible Vapochromism. **Chemistry-a European Journal 2011, 17,** (40), 11102-11106.

Kumar, M.; George, S. J., Green fluorescent organic nanoparticles by self-assembly induced enhanced emission of a naphthalene diimide bolaamphiphile. Nanoscale 2011, 3, (5), 2130-2133.

Kumar, N; Jagadeesan, D; Pillai, PB; Chacko, M; Eswaramoorthy, M; Sundaresan, A; Ferromagnetism in thin-walled hollow spheres of non-magnetic inorganic materials. **Chemical Physics Letters 2011, 504,** (4-6), 189-192.

Kumar, N; Raidongia, K; Mishra, AK; Waghmare, UV; Sundaresan, A; Rao, CNR, Synthetic approaches to borocarbonitrides, BCxN (x=1-2). **Journal of Solid State Chemistry 2011, 184,** (11), 2902-2908.

Kumar, N; Subrahmanyam, KS; Chaturbedy, P; Raidongia, K; Govindaraj, A; Hembram, KPSS; Mishra, AK; Waghmare, UV; Rao, CNR, Remarkable Uptake of CO_2 and CH_4 by Graphene-Like Borocarbonitrides, BxCyNz. **Chemsuschem 2011, 4,** (11), 1662-1670.

Kumar, N; Sundaresan, A; Rao, CNR, Rare earth niobium oxynitrides, LnNbON(2-delta) (Ln = Y, La, Pr, Nd, Gd, Dy): Synthesis, structure and properties. **Materials Research Bulletin 2011, 46,** (11), 2021-2024.

Kumar, P; Panchakarla, LS; Rao, CNR; Laser-induced unzipping of carbon nanotubes to yield graphene nanoribbons. **Nanoscale 2011, 3,** (5), 2127-2129.

Larson, AM; Hsu, BB; Rautaray, D; Haldar, J; Chen, J; Klibanov, AM, Hydrophobic Polycationic Coatings Disinfect Poliovirus and Rotavirus Solutions. **Biotechnology and Bioengineering 2011, 108,** (3), 720-723.

Late, DJ; Ghosh, A; Chakraborty, B; Sood, AK; Waghmare, UV; Rao, CNR, Molecular charge-transfer interaction with single-layer graphene. **Journal of Experimental Nanoscience 2011, 6,** (6), 641-651.

Late, DJ; Liu, B; Matte, HSSR; Rao, CNR; Dravid, VP; Rapid Characterization of Ultrathin Layers of Chalcogenides on SiO2/Si Substrates. **Advanced Functional Materials 2012, 22,** (9), 1894-1905.

Mahata, P; Sarma, D; Madhu, C; Sundaresen, A; Natarajan, S, $CoMn_2O_4$ spinel from a MOF: synthesis, structure and magnetic studies. **Dalton Transactions 2011, 40,** (9), 1952-1960.

Maitra, U; Das, B; Kumar, N; Sundaresan, A; Rao, CNR, Ferromagnetism Exhibited by Nanoparticles of Noble Metals. **ChemPhysChem 2011, 12,** (12), 2322-2327.

Maitra, U; Jain, A; George, SJ; Rao, CNR; Tunable fluorescence in chromophore-functionalized nanodiamond induced by energy transfer. **Nanoscale 2011, 3,** (8), 3192-3197.

Maity, D; Govindaraju, T; Highly Selective Colorimetric Chemosensor for Co_{2+}. **Inorganic Chemistry 2011, 50,** (22), 11282-11284.

Maity, D; Govindaraju, T; Naphthaldehyde-Urea/Thiourea Conjugates as Turn-On Fluorescent Probes for Al_{3+} Based on Restricted C=N Isomerization. **European Journal of Inorganic Chemistry 2011, (36),** 5479-5485.

Maity, D; Govindaraju, T; Highly Selective Visible and Near-IR Sensing of Cu_{2+} Based on Thiourea–Salicylaldehyde Coordination in Aqueous Media. **Chemistry – A European Journal 2011, 17,** (5), 1410-1414.

Maity, D; Govindaraju, T; A differentially selective sensor with fluorescence turn-on response to Zn2+ and dual-mode ratiometric response to Al3+ in aqueous media. **Chemical Communications 2012, 48,** (7), 1039-1041.

Maity, D.; Manna, A. K.; Karthigeyan, D.; Kundu, T. K.; Pati, S. K.; Govindaraju, T., Visible-Near-Infrared and Fluorescent Copper Sensors Based on Julolidine Conjugates: Selective Detection and Fluorescence Imaging in Living Cells. **Chemistry-a European Journal 2011, 17,** (40), 11152-11161.

Mandal, P; Bhadram, VS; Sundarayya, Y; Narayana, C; Sundaresan, A; Rao, CNR; Spin-Reorientation, Ferroelectricity, and Magnetodielectric Effect in YFe1-xMnxO3(0.1≤x≤0.40). **Physical Review Letters 2011, 107,** (13), 137202.

Mandal, P; Bhat, SS; Sundarayya, Y; Sundaresan, A; Rao, CNR; Caignaert, V; Raveau, B; Suard, E; Structure and complex magnetic behavior of disordered perovskite $(Bi_{0.5}Sr_{0.5})(Fe_{0.5}Mn_{0.5})O_3$. **RSC Advances 2011, 2,** (1), 292-297.

Manna, AK; Pati, SK; Tunable Electronic and Magnetic Properties in BxNyCz Nanohybrids: Effect of Domain Segregation. **Journal of Physical Chemistry C 2011,** 115, (21), 10842-10850.

Matte, HSSR; Plowman, B; Datta, R; Rao, CNR, Graphene analogues of layered metal selenides. **Dalton Transactions 2011, 40,** (40), 10322-10325.

Matte, HSSR; Subrahmanyam, KS; Rao, KV; George, SJ; Rao, CNR; Quenching of fluorescence of aromatic molecules by graphene due to electron transfer. **Chemical Physics Letters 2011, 506,** (4-6), 260-264.

Minoia, A; Guo, Z; Xu, H; George, SJ; Schenning, APHJ; De Feyter, S; Lazzaroni, R; Assessing the role of chirality in the formation of rosette-like supramolecular assemblies on surfaces. **Chemical Communications 2011, 47,** (39), 10924-10926.

Mohakud, S; Hijii, K; Miyashita, S; Pati, SK, Effect of Dzyaloshinskii–Moriya interactions on Kagome antiferromagnetic clusters. **Journal of Physics and Chemistry of Solids 2012, 73,** (2), 374-383.

Moses, K; Panchakarla, LS; Matte, HSSR; Govindarao, B; Rao, CNR; Synthesis, characterization and spectroscopy of composites of graphene with CdSe and CdS nanoparticles. **Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry 2011, 50,** (9-10), 1239-1247.

Nagaraja, CM; Haldar, R; Maji, TK; Rao, CNR; Chiral Porous Metal Organic Frameworks of Co(II) and Ni(II): Synthesis, Structure, Magnetic Properties, and CO_2 Uptake. **Crystal Growth & Design 2012, 12,** (2), 975-981.

Nagaraja, CM; Kumar, N; Maji, TK; Rao, CNR, Amine-Templated Cobalt(II) Coordination Polymer Exhibiting Novel Magnetic Properties: Effect of Dehydration. **European Journal of Inorganic Chemistry 2011, 2011, (13),** 2057-2063.

Nagaraja, CM; Maji, TK; Rao, CNR; Synthesis, structure and magnetic properties of two organically-templated coordination polymers, $\{[EDAH_2][M_1M_2F_2(SO_4)_2(H_2O)_2]\}_n$ ($M_1 = M_2 = Ni^{II}$ and $M_1 = Co_{II}$, $M_2 = Ni^{II}$). **Inorganica Chimica Acta 2012, 389,** (0), 85-89.

Nandi, GC; Singh, MS; Ila, H; Junjappa, H; Highly Regioselective One-Pot, Three-Component Synthesis of 1-Aryl-3,4-Substituted/Annulated-5-(Cycloamino)/(Alkylamino)pyrazoles from beta-Oxodithioesters. **European Journal of Organic Chemistry 2012, (5),** 967-974.

Narayanaswamy, N; Govindaraju, T; Aldazine-based colorimetric sensors for Cu_{2+} and Fe_{3+}. **Sensors and Actuators B: Chemical 2012, 161,** (1), 304-310.

Narayanaswamy, N; Maity, D; Govindaraju, T; Reversible fluorescence sensing of Zn_{2+} based on pyridine-constrained bis(triazole-linked hydroxyquinoline) sensor. **Supramolecular Chemistry 2011, 23,** (10), 703-709.

Pandeeswar, M; Avinash, MB; Govindaraju, T; Chiral Transcription and Retentive Helical Memory: Probing Peptide Auxiliaries Appended with Naphthalenediimides for Their One-Dimensional Molecular Organization. **Chemistry-a European Journal 2012, 18,** (16), 4818-4822.

Parida, P; Pati, SK; Painelli, A; Negative differential conductance in nanojunctions: A current constrained approach. **Physical Review B 2011, 83,** (16), 165404.

Peter, SC; Disseler, SM; Svensson, JN; Carretta, P; Graf, MJ, Yb4LiGe4 - A Yb mixed valent Zintl phase with strong electronic correlations. **Journal of Alloys and Compounds 2012, 516,** 126-133.

Peter, SC; Kanatzidis, MG, ThSi2 Type Ytterbium Disilicide and its Analogues YbTxSi2–x (T = Cr, Fe, Co). **Zeitschrift für anorganische und allgemeine Chemie 2012, 638,** (2), 287-293.

Peter, SC; Malliakas, CD; Nakotte, H; Kothapilli, K; Rayaprol, S; Schultz, AJ; Kanatzidis, MG; The polygallides: $Yb_3Ga_7Ge_3$ and $YbGa_4Ge_2$. **Journal of Solid State Chemistry 2012, 187,** 200-207.

Peter, SC; Rayaprol, S; Francisco, MC; Kanatzidis, MG; Crystal Structure and Properties of $Yb_5Ni_4Ge_{10}$. **European Journal of Inorganic Chemistry 2011, (26),** 3963-3968.

Rao, CNR; The two faces of chemistry in the developing world. **Nature Chemistry 2011, 3,** (9), 678-680.

Rao, CNR; Subrahmanyam, KS; Matte, HSSR; Govindaraj, A; Graphene: Synthesis, Functionalization and Properties. **Modern Physics Letters B 2011, 25,** (7), 427-451.

Rao, CNR; Subrahmanyam, KS; Matte, HSSR; Maitra, U; Moses, K; Govindaraj, A; Graphene: Synthesis, Functionalization and Properties. **International Journal of Modern Physics B 2011,** 25, (30), 4107-4143.

Rao, KV; Datta, KKR; Eswaramoorthy, M; George, SJ; Light-Harvesting Hybrid Hydrogels: Energy-Transfer-Induced Amplified Fluorescence in Noncovalently Assembled Chromophore-Organoclay Composites. **Angewandte Chemie-International Edition 2011, 50,** (5), 1179-1184.

Rao, KV; Datta, KKR; Eswaramoorthy, M; George, SJ**;** Light-Harvesting Hybrid Assemblies. **Chemistry-a European Journal 2012, 18,** (8), 2184-2194.

Rao, KV; Haldar, R; Kulkarni, C; Maji, TK; George, SJ; Perylene Based Porous Polyimides: Tunable, High Surface Area with Tetrahedral and Pyramidal Monomers. **Chemistry of Materials 2012, 24,** (6), 969-971.

Rao, KV; Mohapatra, S; Kulkarni, C; Maji, TK; George, SJ; Extended phenylene based microporous organic polymers with selective carbon dioxide adsorption. **Journal of Materials Chemistry 2011, 21,** (34), 12958-12963.

Rao, KV; Mohapatra, S; Maji, TK; George, SJ; Guest-Responsive Reversible Swelling and Enhanced Fluorescence in a Super-Absorbent, Dynamic Microporous Polymer. **Chemistry-a European Journal 2012, 18,** (15), 4505-4509.

Roul, B; Rajpalke, MK; Bhat, TN; Kumar, M; Kalghatgi, AT; Krupanidhi, SB; Kumar, N; Sundaresan, A; Experimental evidence of Ga-vacancy induced room temperature ferromagnetic behavior in GaN films. **Applied Physics Letters 2011, 99,** (16).

Rout, CS; Kumar, A; Kumar, N; Sundaresan, A; Fisher, TS; Room-temperature ferromagnetism in graphitic petal arrays. **Nanoscale 2011, 3,** (3), 900-903.

Saha, R; Shireen, A; Bera, AK; Shirodkar, SN; Sundarayya, Y; Kalarikkal, N; Yusuf, SM; Waghmare, UV; Sundaresan, A; Rao, CNR; Structure and magnetic properties of the $Al_{1-x}Ga_xFeO_3$ family of oxides: A combined experimental and theoretical study. **Journal of Solid State Chemistry 2011, 184,** (3), 494-501.

Saha, R; Shireen, A; Shirodkar, SN; Singh, MS; Waghmare, UV; Sundaresan, A; Rao, CNR; Phase Transitions of $AlFeO_3$ and $GaFeO_3$ from the Chiral Orthorhombic (Pna21) Structure to the Rhombohedral ($R\bar{3}c$) Structure. **Inorganic Chemistry 2011, 50,** (19), 9527-9532.

Saha, R; Shireen, A; Shirodkar, SN; Waghmare, UV; Sundaresan, A; Rao, CNR; Effect of Cr and Mn ions on the structure and magnetic properties of $GaFeO_3$: Role of the substitution site. **Journal of Solid State Chemistry 2011, 184,** (9), 2353-2359.

Samanta, PK; Periyasamy, G; Manna, AK; Pati, SK; Computational studies on structural and optical properties of single-stranded DNA encapsulated silver/gold clusters. **Journal of Materials Chemistry 2012, 22,** (14), 6774-6781.

Sasidharan, A; Panchakarla, LS; Chandran, P; Menon, D; Nair, S; Rao, CNR; Koyakutty, M; Differential nano-bio interactions and toxicity effects of pristine versus functionalized graphene. **Nanoscale 2011, 3, (6),** 2461-2464.

Shireen, A; Saha, R; Mandal, P; Sundaresan, A; Rao, CNR; Multiferroic and magnetodielectric properties of the $Al_{1-x}Ga_xFeO_3$ family of oxides. **Journal of Materials Chemistry 2010, 21,** (1), 57-59.

Shivaprasad, M; Govindaraju, T; Rhodamine based bright red colourimetric and turn-on fluorescence chemosensor for selective detection of Cu_{2+}. **Materials Technology 2011, 26,** (4), 168-172.

Singh, OM; Devi, LR; Singh, TP; Ila, H; Intramolecular cyclocondensation of alpha-oxoketene N,N-, N,S- and N,O-acetals: synthesis of novel pyrido[1,2-a]pyrimidinium tetrafluoroborates. **Arkivoc 2011,** 297-309.

Singh, PP; Yadav, AK; Ila, H; Junjappa, H; A Novel Radical Cyclization Approach to Thieno-Fused Heterocycles. **European Journal of Organic Chemistry 2011, (20-21),** 4001-4007.

Subbarao, U; Peter, SC; Crystal Structure of YbCu6In6 and Mixed Valence Behavior of Yb in YbCu6â€“xIn6+x (x = 0, 1, and 2) Solid Solution. **Inorganic Chemistry 2012, 51,** (11), 6326-6332.

Sundarayya, Y; Mandal, P; Sundaresan, A; Rao, CNR; Mossbauer spectroscopic study of spin reorientation in Mn-substituted yttrium orthoferrite. **Journal of Physics-Condensed Matter 2011, 23,** (43).

Tanaka, Y; Yanagisawa, T; Crisan, A; Shirage, PM; Iyo, A; Tokiwa, K; Nishio, T; Sundaresan, A; Terada, N; Domains in multiband superconductors. **Physica C-Superconductivity and Its Applications 2011, 471,** (21-22), 747-750.

Varghese, N; Rao, CNR; Magnetic nanofilms of nickel prepared at the liquid-liquid interface. **Materials Research Bulletin 2011, 46,** (9), 1500-1503.

Viswanatha, R; Brovelli, S; Pandey, A; Crooker, SA; Klimov, VI; Copper-Doped Inverted Core/Shell Nanocrystals with "Permanent" Optically Active Holes. **Nano Letters 2011, 11,** (11), 4753-4758.

Viswanatha, R; Pietryga, JM; Klimov, VI; Crooker, SA; Spin-Polarized Mn_{2+} Emission from Mn-Doped Colloidal Nanocrystals. **Physical Review Letters 2011,** 107, (6).

Weight, AK; Haldar, J; de Cienfuegos, LA; Gubareva, LV; Tumpey, TM; Chen, J; Klibanov, AM; Attaching Zanamivir to a Polymer Markedly Enhances Its Activity Against Drug-resistant Strains of Influenza a Virus. J**ournal of Pharmaceutical Sciences 2011, 100,** (3), 831-835.

Yamijala, SRKCS; Periyasamy, G; Pati, SK; Computational Studies on Structural and Excited-State Properties of Modified Chlorophyll f with Various Axial Ligands. **Journal of Physical Chemistry A 2011, 115,** (44), 12298-12306.

THEORETICAL SCIENCES UNIT

Das, Subir K; Roy, Sutapa; Majumder, Suman and Ahmad, Shaista; Finite-size effects in dynamics: Critical vs coarsening phenomena. **Europhysics Letters,** (2012).

Das, Subir K; Spiral Dynamics in the Complex Ginzburg-Landau Equation: Disorder vs. Freezing. **Europhysics Letters 97,** 46006 (2012).

Jaiswal, Prabhat K; Puri, Sanjay and Das, Subir K; Hydrodynamic Crossovers in Surface-Directed Spinodal Decomposition and Surface Enrichment. **Europhysics Letters 97,** 16005 (2012).

Subir K. Das and Kurt Binder, Thermodynamic properties of a symmetrical binary mixture in the coexistence region. **Physical Review E 84,** 061607 (2011).

Das, Subir K; and Binder, Kurt; Universal Critical Behavior of Curvature Dependent Interfacial Tension. **Physical Review Letters 107,** 235702 (2011).

Das, Subir K; Kim, Young C; and Fisher, Michael E; When is a Conductor not Perfect? Sum Rules fail under Critical Fluctuations. **Physical Review Letters 107,** 215701 (2011).

Majumder, Suman; and Das, Subir K; Universality in Fluid Domain Coarsening: The case of vapor-liquid transition. **Europhysics Letters 95,** 46002 (2011).

Binder, Kurt; Block, Benjamin J; Das, Subir K; Virnau, Peter; and Winter, David; Monte Carlo Methods for Estimating Interfacial Free Energies and Line Tensions. **Journal of Statistical Physics 144,** 690 - 729 (2011).

Majumder, Suman; and Das, Subir K; Diffusive Domain Coarsening : Early-Time Dynamics and Finite-Size Effects. **Physical Review E 84,** 021110 (2011).

Das, Subir K; and Binder, Kurt; Does Young's equation hold on the nanoscale? A Monte Carlo test for the binary Lennard-Jones fluid, submitted. **Europhysics Letters 92,** 26006 (2010).

Das, Subir K; and Binder, Kurt; Computer Simulations of Phase Diagrams, Critical Phenomena and Interfacial Properties of fluids. **AIP Conference Proceedings 1319,** 129 - 140 (2010).

Block, Benjamin J; Das, Subir K; Oettel, Martin; Virnau, Peter; and Binder, Kurt; Curvature Dependence of Surface Free Energy of Liquid Drops and Bubbles: A Simulation Study. **Journal of Chemical Physics 133,**

Jaiswal, Prabhat K; Puri, Sanjay; and Das, Subir K; Kinetics of Surface Enrichment: A Molecular Dynamics Study. **Journal of Chemical Physics (Research Highlight) 133,** 154901 (2010).

Ahmad, Shaista; Das, Subir K; and Puri, Sanjay; Kinetics of Phase Separation in Fluids: A Molecular Dynamics Study. **Rapid Communication Physical Review E 82,** 040107 (2010).

Jaiswal, Prabhat K; Puri, Sanjay; and Das, Subir K; Kinetics of Surface Enrichment: A Molecular Dynamics Study. **Journal of Chemical Physics (Research Highlight) 133,** 154901 (2010).

Majumder, Suman; and Das, Subir K; Domain coarsening in two dimensions: Conserved dynamics and finite-size scaling. **Rapid Communication Physical Review E 81,** 050102 (2010).

Binder, Kurt; Puri, Sanjay; Das, Subir K; and Horbach, Juergen; Phase Separation in Confined Geometries. **Journal of Statistical Physics 138,** 51 - 84 (2010).

Jain, Kavita; Number of adaptive steps to a local fitness peak. **EPL 96,** 58006 (2011)

Jain, Kavita; Seetharaman, Sarada; Multiple adaptive substitutions during evolution in novel environments. **Genetics 189,** 1029 (2011)

Jain, Kavita; and Seetharaman, Sarada; Nonlinear deterministic equations in biological evolution. **Journal of Nonlinear Mathematical Physics 18 321** (2011)

Jain, Kavita. Extreme value distributions for weakly correlated fitnesses in block model. **Journal of Statistical Mechanics P04020** (2011)

Jain, Kavita; Krug, Joachim; Park, Su-Chan; Evolutionary advantage of small populations on complex fitness landscapes. **Evolution 65,** 1945 (2011)

Seetharaman, Sarada; Jain, Kavita; Evolutionary dynamics on strongly correlated fitness landscapes. **Physical Review E 82,** 031109 (2010).

24. Jain, Kavita; Time to fixation in the presence of recombination. **Theoretical Population Biology 77,** 23 (2010)

25. Marathe, M; Lagoute, J; Repain, V; Rousset, S; and Narasimhan, S; Spin-Polarized Surface States on Fe-Deposited Au(111) surface: A theoretical Study. **Surface Science,** http://dx.doi.org/10.1016/j.susc.2012.02.014 (2012).

26. Mehendale, S; Marathe, M; Girard, Y; Repain, V; Chacon, C; Lagoute, J; Rousset, S; and Narasimhan, S; Prediction of Reconstruction in Heteroepitaxial Systems Using the Frenkel-Kontorova Model. **Physical Review B, 84,** 195458 (2011).

Odell, A; Delin, A; Johansson, B; Ulman, K; Narasimhan, S; Rungger, I; and Sanvito, S; Comparison between s- and d-electron mediated transport in a photoswitching dithienylethene molecule using ab initio transport methods. **Physical Review B, 84,** 165402 (2011).

Delga, A; Lagoute, J; Repain, V; Chacon, C; Girard, Y; Marathe, M; Narasimhan, S; and Rousset, S; Electronic Properties of Fe Clusters on a Au(111) Surface. **Physical Review B, 84,** 035416 (2011).

Imam M. and Narasimhan S., Magnetism of surface alloys of the type MxN1- x/Rh(1 1 1). **Journal of Magnetism and Magnetic Materials, 323,** 1873 – (2011).

Mammen, N; Narasimhan, S; and de Gironcoli, S; Tuning the Morphology of Gold Clusters by Substrate Doping. **Journal of the American Chemical Society, 133,** 2801 (2011).

Hatt, A; Melot, B; and Narasimhan, S; Harmonic and anharmonic properties of Fe and Ni: Thermal expansion, exchange-correlation errors, and magnetism. **Physical Review B, 82,** 134418 (2010).

Mehendale, S; Girard, Y; Repain, V; Chacon, C; Lagoute, J; Rousset, S; Marathe, M; and Narasimhan, S; Ordered Surface Alloy of Bulk-Immiscible Components Stabilized by Magnetism. **Physical Review Letteres, 105,** 056101 (2010) (Editors' Choice).

Prevot, G; Girard, Y; Repain, V; Rousset, S; Coati, A; Garreau, Y; Paul, J; Mammen, N; and Narasimhan, S; Elastic Displacements and Step Interactions on Metallic Surfaces: GIXD and ab initio study of Au(332). **Physical Review B, 81,** 075415 (2010).

Subrahmanyam, KS; Manna, Arun K; Pati, Swapan K; and Rao, CNR; A study of graphene decorated with metal nanoparticles. **Chemical Physical Letters, 497,** 70, 2010.

Manna, Arun K; and Swapan, K Pati; Doping single-walled carbon nanotubes through molecular charge-transfer: a theoretical study. **Nanoscale, 2,** 1190, 2010.

Mohakud, S; Andrews, Alex P; and Pati, Swapan K; Ambipolar charge transport in α-oligofurans: A theoretical study. **Journal of Physical Chemistry. C, 114,** 20436, 2010.

Sudipta, Dutta; and Pati, Swapan K; Novel Properties of Graphene Nanoribbons: A Review. **Journal of Materials Chemistry, 20,** 8207, 2010.

Mallajosyula, Sairam S; and Swapan, K. Pati; Towards DNA Conductivity : A Theoretical Perspective: A Review. **Journal of Physical Chemistry Letters, 1,** 1881, 2010.

Nagaraja, CM, Behera, JN; Maji, Tapas K; Swapan, K Pati; and Rao, CNR; Organically-templated Kagomé compounds containing two transition metal ions. **Dalton Transactions, 39,** 6947, 2010.

Matte, Ramakrishna HSS; Gomathi, A; Manna, Arun K; Late, Dattatray J; Datta, Ranjan; Swapan, K Pati; and Rao, CNR; Graphene analogues of MoS2 and WS2. **Angewandte Chemie International Ed., 49,** 4059, 2010.

Dutta, Sudipta; and Swapan, K Pati; Edge reconstructions induces magnetic and metallic behavior in zigzag graphene nanoribbons. **Carbon, 48,** 4409, 2010.

Datta, A; Mallajosyula, SS; and Pati, Swapan K; Computational Studies on Molecules with Unusual Aromaticity: What to Expect?. **Aromaticity and Metal Clusters,** ed. P. K. Chattaraj (CRC Press, Taylor & Francis Group) 69, 2010.

Parida, Prakash; Kundu, Anasuya; and Pati, Swapan K; Organometallic Vanadium-Anthracene and its B-N Analogue: Efficient Spin Filters. **Physical Chemistry Chemical Physics, 12,** 6924, 2010.

Pandith, AH; and Pati, Swapan K; Conformational Analysis and Vibrational Circular Dichroism of trisethylenediamineruthenium‖ Complex : A Theoretical Study. **Journal of Physical Chemistry A, 114,** 87, 2010.

Ghosh, Dibyajyoti; Periyasamy, Ganga; and Pati, Swapan K; Density Functional Theoretical investigation of the aromatic nature of the BN substituted Benzene and four ring polyaromatic hydrocarbons. **Physical Chemistry Chemical Physics, 13,** 20627, 2011.

Maity, Debabrata; Manna, Arun K; Karthigeyan, D; Tapas, Kundu K; Pati, Swapan K; and Govindaraju, T; Visible-near infrared and fluorescent copper sensors based on julolidine conjugates: selective detection and fluorescence imaging in living cells. **Chemistry: A European Journal, 17,** 11152, 2011.

Yamijala, Sharma; Periyasamy, Ganga; and Pati, Swapan K; Computational Studies on Structural and Excited State Properties of Chlorophyll f with various axial ligands. **Journal of Physical Chemistry. A, 115,** 12298, 2011.

Manna, Arun K; Pati, Swapan K; Doping of Graphene: A Computational Study. **Graphene and its Novel Attributes,** ed. S. K. Pati, T. Enoki, C. N. R. Rao (World Scientific Publishing Co. Pte. Ltd., Singapore), 59, 2011.

Pati, Swapan K; Enoki, T; and Rao, CNR; edited, **Graphene and its fascinating attributes** (World Scientific Publishing Co. Pte. Ltd. Singapore: ISBN: 13-978-981-4329-35-4, 2011.

Das, Barun; Choudhury, Biswajit; Gomathi, A; Manna, Arun K; Pati, Swapan K; and Rao CNR; Interaction of inorganic nanoparticles with graphene, Chemistry Physics. **Chemistry, 12,** 937, 2011.

Sissa, C; Manna, Arun K; Terenziani, F; Painelli, A; and Pati, Swapan K; Beyond the Förster formulation for resonance energy transfer: the role of dark states. **Physical Chemistry Chemical Physics, 13,** 12734, 2011.

Manna, Arun K; and Pati, Swapan K; Tunable Electronic and Magnetic Properties in BxNyCz Nanohybrids: Effect of Domain Segregation. **Journal of Physical Chemistry C, 115,** 10842, 2011.

Basheer, Ershaad Ahamed; Parida, Prakash; and Pati, Swapan K; Electronic and magnetic properties of BNC nanoribbons: a detailed computational study. **New Journal of Physics, 13,** 053008, 2011.

Parida Prakash; Pati, Swapan K; and Painelli; Anna; Negative Differential Conductance in Nano-junctions: A Current Constraint Approach. **Physical Review B, 83,** 165404, 2011.

Ghosh, Sandeep; Yamijala, Sharma; Pati, Swapan K; and Rao, CNR; Interaction of Halogen Molecules with SWNTs and Graphene. **RSC Adv. 2, 1181** (2012).

Datta, A; Srirangarajan, A; Waghmare, U V; Ramamurty, U; Surface effects on stacking fault and twin formation in fcc nanofilms: A first-principles study, **Computational Materials Science, 50,** 12, 3342-3345, (2011).

Saha, Rana; Shireen, Ajmala; Shirodkar, Sharmila; Phase Transitions of AlFeO(3) and GaFeO(3) from the Chiral Orthorhombic (Pna2(1)) Structure to the Rhombohedral (R(3)over-barc). **Structure Inorganic Chemistry, 50,** 19, 9527-9532, (2011).

Choudhury, D; Mukherjee, S; Mandal, P; Sundaresan, A; Waghmare, U V; Bhattacharjee, S; Mathieu, R; Lazor, P; Eriksson, O; Sanyal, B; Nordblad, P; Sharma, A; Bhat, SV; Karis, O; Sarma, DD; Tuning of dielectric properties and magnetism of SrTiO(3) by site-specific doping of Mn.**Physical Review B, 84,** 12, 125124, (2011).

Saha, Rana; Shireen, Ajmala; Shirodkar, Sharmila N; Waghmare, Umesh V; Sundaresan, A; Rao, CNR; Effect of Cr and Mn ions on the structure and magnetic properties of GaFeO(3): Role of the substitution site. **Journal of Solid State Chemistry, 184,** 9, 2353-2359, (2011).

Chakraborty, Indrani; Carvalho, Daniel; Shirodkar, Sharmila N; Lahiri, Sandeep; Bhattacharyya, Somnath; Banerjee, Rajarshi; Waghmare, Umesh; Ayyub, Pushan; Novel hexagonal polytypes of silver: growth, characterization and first-principles calculations. **Journal of Physics-Condensed Matter, 23,** 32, 325401, (2011).

Grau-Crespo, Ricardo; de Leeuw, Nora H; Hamad, Said; Waghmare, Umesh V; Phase separation and surface segregation in ceria-zirconia solid solutions. **Proceedings of the Royal Society a-Mathematical Physical and Engineering Sciences, 467,** 2131, 1925-1938, (2011).

Dutta, Gargi; Gupta, Asha; Waghmare, Umesh V; Hegde, MS; CO adsorption on ionic Pt, Pd and Cu sites in Ce(1-x) M(x)O(2-delta) (M = Pt(2+), Pd(2+), Cu(2+)). **Journal of Chemical Sciences, 123,** 4, 509-516, (2011).

Kumar, Pradeep; Bera, Achintya; Muthu, DVS; Kumar, Anil; Waghmare, UV; Harnagea, L; Hess, C; Wurmehl, S; Singh, S; Buechner, B; Sood, AK; Raman evidence for the superconducting gap and spin-phonon coupling in the superconductor Ca(Fe(0.95)Co(0.05))(2)As(2). **Journal of Physics-Condensed Matter, 23,** 25, 255403, (2011).

Sanyal, Suchismita; Waghmare, Umesh V; Ruud, James A; Adsorption of water on TiN (100), (110) and (111) surfaces: A first-principles study. **Applied Surface Science, 257,** 15, 6462-6467, (2011).

Saha, B; Sands, TD; Waghmare, UV; First-principles analysis of ZrN/ScN metal/semiconductor superlattices for thermoelectric energy conversion. **Journal of Applied Physics,109,**8, 083717, (2011).

Saha, B; Sands, TD; Waghmare, UV; Electronic structure, vibrational spectrum, and thermal properties of yttrium nitride: A first-principles study. **Journal of Applied Physics, 109,** 7, 073720, (2011).

Sanyal, S; Waghmare, UV; Ruud, JA; Adsorption of water on TiN (100), (110) and (111) surfaces: A first-principles study. **Applied Surface Science, 257,** 15, 6462-6467, (2011).

Dileep, K; Panchakarla, LS; Balasubramanian, K; Waghmare, UV, Datta, R; Electron energy loss spectroscopy of ZnO nanocrystals with different oxygen vacancy concentrations. **Journal of Applied Physics, 109,** 6, 063523, (2011).

Das, H; Waghmare, UV; Saha-Dasgupta, T; Piezoelectrics by design: A route through short-period Perovskite superlattices. **Journal of Applied Physics, 109,** 6, 066107, (2011).

Saha, R; Shireen, A; Bera, AK; Shirodkar, Sharmila N; Sundarayya, Y; Kalarikkal, N; Yusuf, SM; Waghmare, UV; Sundaresan, A; Rao, CNR; Structure and magnetic properties of the Al1-xGaxFeO3 family of oxides: A combined experimental and theoretical study. **Journal of Solid State Chemistry, 184,** 3, 494-501, (2011)

Pundlik, SS; Kayanaraman, K; Waghmare, UV; First-Principles Investigation of the Atomic and Electronic Structure and Magnetic Moments in Gold Nanoclusters. **Journal of Physical Chemistry C, 115,** 10, 3809-3820, (2011)

Subrahmanyam, KS; Kumar, P; Maitra, U; Govindaraj, A; Hembram, KPSS; Waghmare, UV; Rao, CNR; Chemical storage of hydrogen in few-layer graphene. **Procedings of the National Academy of Sciences of the United States of America, 108,** 7, 2674-2677, (2011).

Late, DJ; Maitra, U; Panchakarla, LS; Waghmare, UV; Rao, CNR; Temperature effects on the Raman spectra of graphenes: dependence on the number of layers and doping. **Journal of Physics-Condensed Matter, 23,** 5, 055303, (2011).

Venu, K; Kanuri, S; Raidongia, K; Hembram, KPSS; Waghmare, UV; Datta, R; Band gap and chemically ordered domain structure of a graphene analogue BxCyNz. **Solid State Communications, 150,** 45-46, 2262-2265, (2010).

Dutta, G; Saha, SK; Waghmare, UV; Effects of Zr and Ti doping on the dielectric response of CeO2: A comparative first-principles study. **Solid State Communications, 150,** 41-42, 2020-2022, (2010).

Choudhury, D; Hazarika, A; Venimadhav, A; Kakarla, C; Delaney, KT; Devi, S; Mondal, P; Nirmala, R; Gopalakrishnan, J; Spaldin, NA; Waghmare, UV; Sarma, DD; Electric and magnetic polarizabilities of hexagonal Ln(2)CuTiO(6)(Ln = Y, Dy, Ho, Er, and Yb). **Physical Review B, 82,**13, 134203, (2010).

Pradhan, GK; Kumar, A; Deb, SK; Waghmare, UV; Narayana, C; Elastic and structural instability of cubic Sn3N4 and C3N4 under pressure. **Physical Review B, 82,** 14, 144112, (2010)

Smith, KC; Fisher, TS; Waghmare, UV; Grau-Crespo R, Dopant-vacancy binding effects in Li-doped magnesium hydride. **Physical Review B, 82,** 13, 134109, (2010).

Nishimatsu, T; Iwamoto, M; Kawazoe, Y; Waghmare, UV; First-principles accurate total energy surfaces for polar structural distortions of $BaTiO_3$, $PbTiO_3$, and $SrTiO_3$: Consequences for structural transition temperatures. **Physical Review B, 82,** 13, 134106, (2010).

Gupta, A; Waghmare, UV; Hegde, MS; Correlation of Oxygen Storage Capacity and Structural Distortion in Transition-Metal-, Noble-Metal-, and Rare-Earth-Ion-Substituted CeO_2 from First Principles Calculation. **Chemistry of Materials, 22,** 18, 5184-5198, (2010)

Kumar, S; Hembram, KPSS; Waghmare, UV; Intrinsic buckling strength of graphene: First-principles density functional theory calculations. **Physical Review B, 82,** 11, 115411, (2010)

Kumar, A; Kumar, P; Waghmare, UV; Sood, AK; First-principles analysis of electron correlation, spin ordering and phonons in the normal state of $FeSe_{1-x}$. **Journal of Physics-Condensed Matter, 22,** 38, 385701, (2010).

Dzade, NY; Obodo, KO; Adjokatse, SK; Ashu, AC; Amankwah, E; Atiso, CD; Bello, AA; Igumbor, E; Nzabarinda, SB; Obodo, JT; Ogbuu, AO; Femi, OE; Udeigwe, JO; Waghmare, UV; Silicene and transition metal based materials: prediction of a two-dimensional piezomagnet, **Journal of Physics-Condensed Matter, 22,** 37, 375502, (2010)

Kumar A, Waghmare UV, First-principles free energies and Ginzburg-Landau theory of domains and ferroelectric phase transitions in $BaTiO_3$. **Physical Review B, 82,** 5, 054117, (2010)

Sanyal, S; Waghmare, UV; Subramanian, PR; Gigliotti, MFX; First-principles understanding of environmental embrittlement of the Ni/Ni_3Al interface. **Scripta Materialia, 63,** 4, 391-394, (2010)

Das, H; Spaldin, NA; Waghmare, UV; Saha-Dasgupta, T; Chemical control of polar behavior in bicomponent short-period superlattices. **Physical Review B, 81,** 23, 235112, (2010)

Kumar, P; Kumar, A; Saha, S; Muthu, Prakash J; Waghmare, UV; Ganguli, AK; Sood, AK; Temperature-dependent Raman study of a $CeFeAsO_{0.9}F_{0.1}$ superconductor: crystal field excitations, phonons and their coupling. **Journal of Physics-Condensed Matter, 22,** 25, 255402 (2010).

Tripathi, S; Kumar, A; Waghmare, UV; Pandey, D; Effect of $NaNbO_3$ substitution on the quantum paraelectric behavior of $CaTiO_3$. **Physical Review B, 81,** 21, 212101, (2010).

Gupta, A; Kumar, A; Hegde, MS; Waghmare, UV; Structure of $Ce_{1-x}Sn_xO_2$ and its relation to oxygen storage property from first-principles analysis. **Journal of Chemical Physics, 132,** 19, 194702, (2010).

Bhowmick, S; Waghmare, UV; Anisotropy of the Stone-Wales defect and warping of graphene nanoribbons: A first-principles analysis. **Physical Review B, 81,** 15, 155416, (2010).

Choudhury, D; Venimadhav, A; Kakarla, C; Delaney, KT; Devi, PS; Mondal, P; Nirmala, R; Gopalakrishnan, J; Spaldin, NA; Waghmare, UV; Sarma, DD; Unusual dielectric response in B-site size-disordered hexagonal transition metal oxides. **Appl. Phys. Lett, 96,** 16, 162903, (2010)

Kumar, P; Kumar, A; Saha, S; Muthu, DVS; Prakash, J; Patnaik, S; Waghmare, UV; Ganguli, AK; Sood, AK; Anomalous Raman scattering from phonons and electrons of superconducting $FeSe_{0.82}$. **Solid State Communications, 150,** 13-14, 557-560, (2010)

Nag, A; Raidongia, K; Hembram, KPSS; Datta, R; Waghmare, UV; Rao, CNR; Graphene Analogues of BN: Novel Synthesis and Properties. **ACS Nano, 4,** 3,1539-1544, (2010)

Deepak, J; Pradeep, T; Waghmare, UV; Interaction of small gold clusters with carbon nanotube bundles: formation of gold atomic chains. **Journal of Physics-Condensed Matter, 22,** 12, 125301, (2010)

Raidongia, K; Hembram, KPSS; Waghmare, UV; Eswaramoorthy, M; Rao, CNR; Synthesis, Structure, and Properties of Mesoporous B/C/N Microspheres. **Zeitschrift Fur Anorganische Und Allgemeine Chemie, 636,** 1, 30-35, (2010)

Saha, B; Acharya, J; Sands, TD; Waghmare, UV; Electronic structure, phonons, and thermal properties of ScN, ZrN, and HfN: A first-principles study. **Journal of Applied Physics, 107,** 3, 033715 (2010)

Bhattacharjee, J; Waghmare, UV; Wannier orbital overlap population (WOOP), Wannier orbital position population (WOPP) and the origin of anomalous dynamical charges. **Physical Chemistry Chemical Physics, 12,** 7, 1564-1570, (2010).

Dzade, NY; Obodo, KO; Adjokatse, SK; Ashu, AC; Amankwah, E; Atiso, CD; Bello, AA; Igumbor, E; Nzabarinda, SB; Obodo, JT; Ogbuu, AO; Femi, OE; Udeigwe, JO; Waghmare, UV; Silicene and transition metal based materials: prediction of a two-dimensional piezomagnet. **Journal of Physics-Condensed Matter, 22,** 37, 375502, (2010)

Kumar, A; Waghmare, UV; First-principles free energies and Ginzburg-Landau theory of domains and ferroelectric phase transitions in $BaTiO_3$. **Physical Review B, 82,** 5, 054117, (2010)

Sanyal, S; Waghmare, UV; Subramanian, PR; Gigliotti, MFX; First-principles understanding of environmental embrittlement of the Ni/Ni_3Al interface. **Scripta Materialia, 63,** 4, 391-394, (2010)

Das, H; Spaldin, NA; Waghmare, UV; Saha-Dasgupta, T; Chemical control of polar behavior in bicomponent short-period superlattices. **Physical Review B, 81,** 23, 235112, (2010)

Kumar, P; Kumar, A; Saha, S; Muthu; Prakash, J; Waghmare, UV; Ganguli, AK; Sood, AK; Temperature-dependent Raman study of a $CeFeAsO_{0.9}F_{0.1}$ superconductor: crystal field excitations, phonons and their coupling. **Journal of Physics-Condensed Matter, 22,** 25, 255402 (2010)

Tripathi, S;, Kumar; A; Waghmare, UV; Pandey, D; Effect of $NaNbO_3$ substitution on the quantum paraelectric behavior of $CaTiO_3$. **Physical Review B, 81,** 21, 212101, (2010)

Gupta, A; Kumar, A; Hegde, MS; Waghmare, UV; Structure of $Ce_{1-x}Sn_xO_2$ and its relation to oxygen storage property from first-principles analysis. **Journal of Chemical Physics, 132,** 19, 194702, (2010)

Bhowmick, S; Waghmare, UV; Anisotropy of the Stone-Wales defect and warping of graphene nanoribbons: A first-principles analysis. **Physical Review B, 81,** 15, 155416, (2010)

Choudhury, D; Venimadhav, A; Kakarla, C; Delaney, KT; Devi, PS; Mondal, P; Nirmala, R; Gopalakrishnan, J; Spaldin, NA; Waghmare, UV; Sarma, DD; Unusual dielectric response in B-site size-disordered hexagonal transition metal oxides. **Appl. Phys. Lett, 96,** 16, 162903, (2010)

Kumar, P; Kumar, A; Saha, S; Muthu, DVS; Prakash, J; Patnaik, S; Waghmare, UV; Ganguli, AK; Sood, AK; Anomalous Raman scattering from phonons and electrons of superconducting FeSe0.82, **Solid State Communications, 150,** 13-14, 557-560, (2010)

Nag, A; Raidongia, K; Hembram, KPSS; Datta, R; Waghmare, UV; Rao, CNR; Graphene Analogues of BN: Novel Synthesis and Properties. **ACS Nano, 4,** 3,1539-1544, (2010)

Deepak, J; Pradeep, T; Waghmare, UV; Interaction of small gold clusters with carbon nanotube bundles: formation of gold atomic chains. **Journal of Physics-Condensed Matter, 22,** 12, 125301, (2010)

Raidongia, K; Hembram, KPSS; Waghmare, UV; Eswaramoorthy, M; Rao, CNR; Synthesis, Structure, and Properties of Mesoporous B/C/N Microspheres. **Zeitschrift Fur Anorganische Und Allgemeine Chemie, 636,** 1, 30-35, (2010)

Saha, B; Acharya, J; Sands, TD; Waghmare, UV; Electronic structure, phonons, and thermal properties of ScN, ZrN, and HfN: A first-principles study. **Journal of Applied Physics, 107,** 3, 033715 (2010)

Bhattacharjee, J; Waghmare, UV; Wannier orbital overlap population (WOOP), Wannier orbital position population (WOPP) and the origin of anomalous dynamical charges. **Physical Chemistry Chemical Physics, 12,** 7, 1564-1570, (2010)

Tripathi, MN; Waghmare, UV; Ramesh, TN; Kamath, PV; Polytypism and Stacking Disorders in Nickel Hydroxide: A First-Principles Study. **Journal of the Electrochemical Society, 157,** 3, 280-A284 (2010)

Raidongia, K; Nag, A; Hembram, KPSS; Waghmare, UV; Datta, R; Rao, CNR; BCN: A Graphene Analogue with Remarkable Adsorptive Properties. **Chemistry European Journal A, 16,** 149 - 157 (2010).

Vasisht, Vishwas V; Saw, Shibu; and Sastry, Srikanth; Liquid-liquid critical point in supercooled silicon. **Nature Physics** (2011)

Saw, Shibu; Ellegaard, Niels L; Kob, Walter; and Sastry, Srikanth; Computer Simulation Study of the Phase Behavior and Structural Relaxation in a Gel-Former Modeled by Three Body Interactions. **Journal of Chemical Physics, 134,** 164506 (2011)

Sastry, Srikanth; Illuminating Liquid Polymorphism in Silicon (Commentary). **Proc. Natl. Acad. Sci. (US), 107,** 17063 (2010)

Buldyrev S. V., Kumar P., Sastry S., Stanley H. E., and Weiner S., Hydrophobic Collapse and Cold Denaturation in the Jagla Model of Water [Proc. Lausanne CECAM Conference], **Journal of Physical Condensed Matter, 22,** 284109 (2010)

Karmakar, Smarajit; Dasgupta, Chandan; Sastry, Srikanth; Analysis of Dynamic Heterogeneity in a Glass Former from the Spatial Correlations of Mobility. **Physical Review Letters, 105,** 015701 (2010)

Karmakar, Smarajit; Dasgupta, Chandan; Sastry, Srikanth; Comment on "Scaling Analysis of Dynamic Heterogeneity in a Supercooled Lennard-Jones Liquid". **Physical Review Letters, 105,** 019801 (2010)

Maiti, M; Rao, M; Satry, S; Competition between folding and aggregation in a model for protein solutions. **Eur. Phys. J. E, 32,** 217 - 221 (2010).

Chaudhuri, Pinaki; Berthier, Ludovic; Sastry, Srikanth; Jamming Transitions in Amorphous Packings of Frictionless Spheres Occur Over a Continuous Range of Volume fractions. **Physical Review Letters, 104,** 165701 (2010).

Kumar, Pramod; and Vidhyadhiraja, NS; From mixed valence to the Kondo lattice regime. **Journal of Physics: Condensed Matter,** (2011).

Taraphder, A; Koley, S; Vidhyadhiraja, NS; and Laad, Mukul S; Preformed excitonic liquid route to charge density wave in 2H-TaSe2. **Physical Review letters, 106,** 236405 (2011).

Rao, Mallikarjuna K; Thiruvelu, Bhuvana; Radha, B; Kurra, Narendra; Vidhyadhiraja, NS; and Kulkarni, GU; Metallic Conduction in NiS2 Nanocrystalline Structures., **Journal of Physical Chemistry, 115,** 10462 - 10467 (2011).

Barman, H; and Vidhyadhiraja, NS; Transport and Spectra in the half-filled Hubbard model: A dynamical mean-field study., **International Journal of Modern Physics B, 25,** 2461 - 2479 (2011).

Mukhopadhyay, Sabyasachi; Voggu, Rakesh; Rao, CNR, Vidhyadhiraja, NS; and Narayan, KS; Lateral photocurrent scanning of donor and acceptor polymers on graphene coated substrates, **Japanese Journal of Applied Physics, 50,** 061602 (2011).

Parihari, D; Vidhyadhiraja, NS; and Taraphder, A; Field dependent dynamics in the metallic regime of the half-filled Hubbard model, **Journal of Physics: Condensed Matter, 23,** 055602 (2011).

CHEMICAL BIOLOGY UNIT

Biswas, J; Bajaj, A; Bhattacharya S; Membranes of Cationic Gemini Lipids based on Cholesterol with Hydroxyl Headgroups and their Interactions with DNA and Phospholipid. **Journal of Physical Chemistry B, 115,** 478-486, 2011.

Bhattacharya, S, Biswas, J. Vesicle and Stable Monolayer Formation from Simple 'Click' Chemistry Adducts in Water, Langmuir, 27, 1581-1591, 2011.

Biswas, J; Mishra, SK; Kondaiah, P; and Bhattacharya, S; Syntheses, Transfection Efficacy and Cell Toxicity Properties of Novel Cholesterol-based Gemini Lipids having Hydroxyethylated Head group. **Organic and Biomolecular Chemistry, 9,** 4600-4613., 2011.

Bhattacharya, S; Biswas, J; Role of spacer lengths of gemini surfactants in the synthesis of silver nanorods in micellar media. **Nanoscale, 3,** 2924-2930. 2011.

Samanta, SK; Pal, A; Bhattacharya, S; An Insight into Fiber-Solvent mediated Modulation of nano-fibrillar Organogels. **International Journal of Nanoscience, 10,** 547-554. 2011.

Kumari, N; Jha, S; Bhattacharya, S; Colorimetric Probes based on Anthraimidazolediones for Selective Sensing of Fluoride and Cyanide ion via Intramolecular Charge Transfer. **Journal of Organic Chemistry, 76,** 8215-8222, 2011.

Jain, A; Bhattacharya, S; Interaction of G-Quadruplexes with Non-intercalating DNA Minor Groove Binding Ligands. **Bioconjugate Chemistry, 22,** 2355-2368, 2011. [By Invitation].

Bhattacharyya, S; Rajan, RE; Swarupa, Y; Rathore, U; Verma, A; Udaykumar, R; and Varadarajan, R; Design of a non-glycosylated outer domain-derived HIV-1 gp120 immunogen that binds to CD4 and induces neutralizing antibodies. **Journal of Biological Chemistry, 285,** 27100, 2010.

Bommakanti, G; Citron, MP; Hepler, RW; Callahan, C; Heidecker, GJ; Najar, TA; Lu, X; Joyce, JG; Shiver, JW; Casimiro, DR; ter Meulen, J; Liang, X; and Varadarajan, R; Design of an HA2-based Escherichia coli expressed influenza immunogen that protects mice from pathogenic challenge. **Proceedings of National Academy of Sciences USA 107,** 13701, 2010. (see also Commentary on paper by Eckert and Kay in same issue at www.pnas.org/cgi/doi/10.1073/pnas.1008672107).

Indu, S; Kumar, ST; Thakurela, S; Gupta, M; Bhaskara, RM; Ramakrishnan, C; and Varadarajan, R; Disulfide conformation and design at helix N-termini. **Proteins 78,** 1228, 2010.

Indu, S; Kochat, V; Thakurela, S; Ramakrishnan, C; and Varadarajan, R; Conformational analysis and design of cross-strand disulfides in antiparallel beta-sheets. **Proteins 79,** 244, 2011.

Adkar, BV; Tripathi, A; Sahoo, A; Bajaj, K; Goswami, D; Chakrabarti, P; Swarnkar, MK; Gokhale, RS; and Varadarajan, R; Protein model discrimination using mutational sensitivity derived from deep sequencing. **Structure 20,** 371, 2012.

Bhowmik, S; Banerjee, S; Maitra, U; A self-assembled, luminescent europium cholate hydrogel: a novel approach towards lanthanide sensitization; **Chemical Communications, 45,** 8642-8644, 2010.

Das, R; K, Kandanelli, R; Linnanto, J; Bose, K; Maitra, U; Supramolecular Chirality in Organogels: A Detailed Spectroscopic, Morphological, and Rheological Investigation of Gels (and Xerogels) Derived from Alkyl Pyrenyl Urethanes. **Langmuir, 26,** 16141- 16149, 2010.

Ramesh, K; Bhowmik, S; Maitra, U; Functional molecular gels - a brief review. **Journal of the Indian Chemical Society, 88,** 1903-1915, 2011 (special issue on the occasion of Acharya P.C. Ray's 150th birth anniversary)

Banerjee, S; Vidya, VM; Savyasachi, AJ; Maitra, U; Perfluoroalkyl bile esters: A new class of efficient gelators of organic and aqueous- organic media", Supratim Banerjee, V.M. Vidya, A.J. Savyasachi and Uday Maitra. **Journal of Materials Chemistry, 21,** 14693, 2011.

Banerjee, S; Kandanelli, R; Bhowmik, S; Maitra, U; Self-organization of multiple components in a steroidal hydrogel matrix: Design, construction and studies on novel tunable luminescent gels and xerogels. **Soft Matter, 7,** 8207, 2011.

Chakrabarty, A; Maitra, U; Protonation and deprotonation induced organo/hydrogelation: Bile acid derived gelators containing a basic side chain. **Beilstein Journal of Organic Chemistry, 7,** 304, 2011.

CONDENSED MATTER THEORY UNIT

Choudhury, D; Venimadhav, A; Kakarla, C; Delaney, KT; Devi, PS; Mondal, P; Nirmala, R; Gopalakrishnan, J; Spaldin, NA; Waghmare, UV; Sarma, DD; Unusual dielectric response in B-site size-disordered hexagonal transition metal oxides. **Applied Physics Letters, 96(16),** 162903, 2010.

Karmakar, S; Dasgupta, C; Sastry, S; Analysis of Dynamic Heterogeneity in a Glass Former from the Spatial Correlations of Mobility. **Physical Review Letters, 105(1),** 015701, 2010.

Karmakar, S; Dasgupta, C; Sastry, S; Comment on "Scaling Analysis of Dynamic Heterogeneity in a Supercooled Lennard-Jones Liquid". **Physical Review Letters, 105(1),** 019801, 2010.

Kumar, N; Sundaresan, A; On the observation of negative magnetization under zero-field-cooled process. **Solid State Communications, 150(25-26),** 1162-1164, 2010.

Mukherjee, B; Maiti, PK; Dasgupta, C; Sood, AK; Single-File Diffusion of Water Inside Narrow Carbon Nanorings. **ACS Nano, 4(2),** 985-991, 2010.

Perlekar, P; Pandit, R; Turbulence-induced melting of a nonequilibrium vortex crystal in a forced thin fluid film. **New Journal of Physics, 12,** 023033, 2010.

Sahoo, G; Mitra, D; Pandit, R; Dynamo onset as a first-order transition: Lessons from a shell model for magnetohydrodynamics. **Physical Review E, 81(3),** 036317, Part: Part 2, 2010.

Viswanatha, R; Amenitsch, H; Santra, S; Sapra, S; Datar, SS; Zhou, Y; Nayak, SK; Kumar, SK; Sarma, DD; Growth Mechanism of Cadmium Sulfide Nanocrystals. **Journal of Physical Chemistry Letters, 1(1),** 304-308, 2010.

Das, H; Waghmare, UV; Saha-Dasgupta, T; Sarma, DD; Theoretical evidence and chemical origin of the magnetism-dependent electrostructural coupling in La_2NiMnO_6. **Physical Review B, 79(14),** 144403, 2009.

Dasgupta, C; Valls, OT; Hydrodynamics of superfluids confined in blocked rings and wedges. **Physical Review E, 79(1),** 016303 Part: Part 2, 2009.

Dasgupta, C; Valls, OT; Phase diagram of vortex matter in layered superconductors with tilted columnar pinning centers. **Physical Review B, 80(9),** 094517, 2009.

Freericks, JK; Krishnamurthy, HR; Ge, YZ; Liu, AY; Pruschke, T; Theoretical description of time-resolved pump/probe photoemission in TaS2: a single-band DFT plus DMFT(NRG) study within the quasiequilibrium approximation. **Physica Status Solidi B-Basic Solid State Physics, 246(5),** 948-954, 2009.

Freericks, JK; Krishnamurthy, HR; Kato, Y; Kawashima, N; Trivedi, N; Strong-coupling expansion for the momentum distribution of the Bose-Hubbard model with benchmarking against exact numerical results. **Physical Review A, 79(5),** 053631, 2009.

Freericks, JK; Krishnamurthy, HR; Pruschke, T; Theoretical Description of Time-Resolved Photoemission Spectroscopy: Application to Pump-Probe Experiments. **Physical Review Letters, 102(13),** 136401, 2009.

Kikuchi, N; Ehrlicher, A; Koch, D; Kas, JA; Ramaswamy, S; Rao, M; Buckling, stiffening, and negative dissipation in the dynamics of a biopolymer in an active medium. **Proceedings of the National Academy of Sciences of The United States of America, 106(47),** 19776-19779, 2009.

Krishna, C; Yashonath, S; Dependence of self-diffusivity on size of impurity atoms in a face-centred cubic solid: existence of an anomalous maximum. **Molecular Simulation, 35(1-2),** 151-161, 2009.

Kumar, N; Kumar, KV; Classical Langevin dynamics of a charged particle moving on a sphere and diamagnetism: A surprise. **EPL, 86(1),** 17001, 2009.

Kumar, N; Sanyal, D; Sundaresan, A; Defect induced ferromagnetism in MgO nanoparticles studied by optical and positron annihilation spectroscopy. **Chemical Physics Letters, 477(4-6),** 360-364, 2009.

Mukherjee, B; Maiti, PK; Dasgupta, C; Sood, AK; Jump Reorientation of Water Molecules Confined in Narrow Carbon Nanotubes. **Journal of Physical Chemistry B, 113(30),** 10322-10330, 2009.

Mukherjee, B; Maiti, PK; Dasgupta, C; Sood, AK; Reorientation of Water Inside Carbon Nanorings by Large Angular Jumps. **Journal of Nanoscience and Nanotechnology, 9(9),** 5303-5306, 2009.

Panchokarla, LS; Subrahmanyam, KS; Saha, SK; Govindaraj, A; Krishnamurthy, HR; Waghmare, UV; Rao, CNR; Synthesis, Structure, and Properties of Boron- and Nitrogen-Doped Graphene. **Advanced Materials, 21(46),** 4726, 2009.

Pandit, R; Perlekar, P; Ray, SS; Statistical properties of turbulence: An overview. **Pramana-Journal of Physics, 73(1),** SI 157-191, 2009.

Perlekar, P; Pandit, R; Statistically steady turbulence in thin films: direct numerical simulations with Ekman friction. **New Journal of Physics, 11,** 073003, 2009.

Raj, S; Chakraborty, A; Choudhury, D; Sato, Takahashi T; Mahadevan, P; Fujii, J; Vobornik, I; Sarma, DD; Three-dimensional band structure of highly metallic $Na_{0.8}WO_3$ by angle-resolved photoemission spectroscopy. **Physical Review B, 79(3),** 035119, 2009.

Saha, SK; Chandrakanth, RC; Krishnamurthy, HR; Waghmare, UV; Mechanisms of molecular doping of graphene: A first-principles study. **Physical Review B, 80(15),** 155414, 2009.

Santra, PK; Viswanatha, R; Daniels, SM; Pickett, NL; Smith, JM; O'Brien, P; Sarma, DD; Investigation of the Internal Heterostructure of Highly Luminescent Quantum Dot-Quantum Well Nanocrystals. **Journal of the American Chemical Society, 131(2),** 470-477, 2009.

Shenoy, VB; Gupta, T; Krishnamurthy, HR; Ramakrishnan, TV; Long-range Coulomb interactions and nanoscale electronic inhomogeneities in correlated oxides. **Physical Review B, 80(12),** 125121, 2009.

Sudhir, VS; Kumar, N; Phani, YP; Baig, RBN; Chandrasekaran, S; Facile Entry into Triazole Fused Heterocycles via Sulfamidate Derived Azido-alkynes. **Journal of Organic Chemistry, 74(19),** 7588-7591, 2009.

Viswanatha, R; Santra, PK; Sarma, DD; Self Assembly and Electronic Structure of ZnO Nanocrystals. **Journal of Cluster Science, 20(2),** 389-398, 2009.

Zenia, H; Freericks, JK; Krishnamurthy, HR; Pruschke, T; Appearance of "Fragile" Fermi Liquids in Finite-Width Mott Insulators Sandwiched between Metallic Leads. **Physical Review Letters, 103(11),** 116402, 2009.

Das, A; Pisana, S; Chakraborty B; Piscanec, S; Saha, SK; Waghmare, UV; Novoselov, KS; Krishnamurthy, HR; Geim, AK; Ferrari, AC; Sood, AK; Monitoring dopants by Raman scattering in an electrochemically top-gated graphene transistor. **Nature Nanotechnology, 3(4),** 210-215, 2008.

Das, H; Waghmare, UV; Saha-Dasgupta, T; Sarma, DD; Electronic structure, phonons, and dielectric anomaly in ferromagnetic insulating double perovskite La_2NiMnO_6. **Physical Review Letters, 100(18),** 186402, 2008.

Demontis, P; Suffritti, GB; Yashonath, S; Comment on "High-Accuracy Estimation of 'Slow' Molecular Diffusion Rates in Zeolite Nanopores, Based on Free Energy Calculations at an Ultrahigh Temperature". **Journal of Physical Chemistry C,** 112(43), 17030-17031, 2008.

Mukherjee, B; Maiti, PK; Dasgupta, C; Sood, AK. Strongly anisotropic orientational relaxation of water molecules in narrow carbon nanotubes and nanorings. **ACS Nano, 2(6),** 1189-1196, 2008.

Pai, RV; Sheshadri, K; Pandit, R; Phases and transitions in the spin-1 Bose-Hubbard model: Systematics of a mean-field theory. **Physical Review B, 77(1),** 014503, 2008.

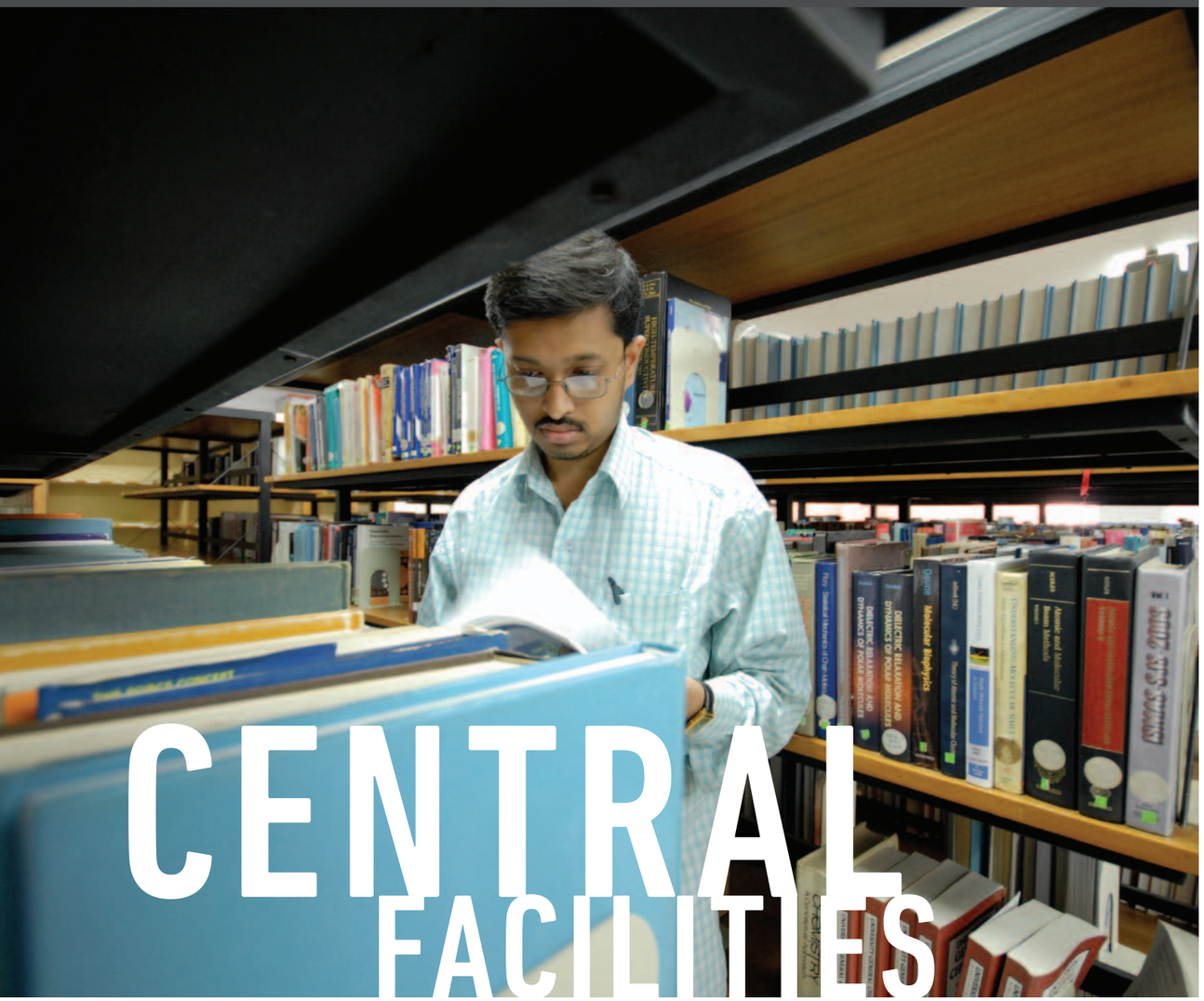
Ray, SS; Mitra, D; Pandit, R; The universality of dynamic multiscaling in homogeneous, isotropic Navier-Stokes and passive-scalar turbulence. **New Journal of Physics, 10,** 033003, 2008.

Saha, SK; Waghmare, UV; Krishnamurthy, HR; Sood, AK; Phonons in few-layer graphene and interplanar interaction: A first-principles study. **Physical Review B, 78(16),** 165421, 2008.

Sanyal, P; Sen Gupta, S; Pakhira, N; Krishnamurthy, HR; Sarma, DD; Ramakrishnan, TV. Theory of the unusual doping and temperature dependence of photoemission spectra in manganites. **EPL, 82(4),** 47010, 2008.

Voggu, R; Kumar, N; Rao, CNR; Dependence of the Properties of Magnetic Nanoparticles on the Interparticle Separation. **Journal of Physical Chemistry C, 112(46),** 17775-17777, 2008.

Yashonath, S; Ghorai, PK; Diffusion in nanoporous phases: Size dependence and levitation effect. **Journal of Physical Chemistry B, 112(3),** 665-686, 2008.



CENTRAL FACILITIES

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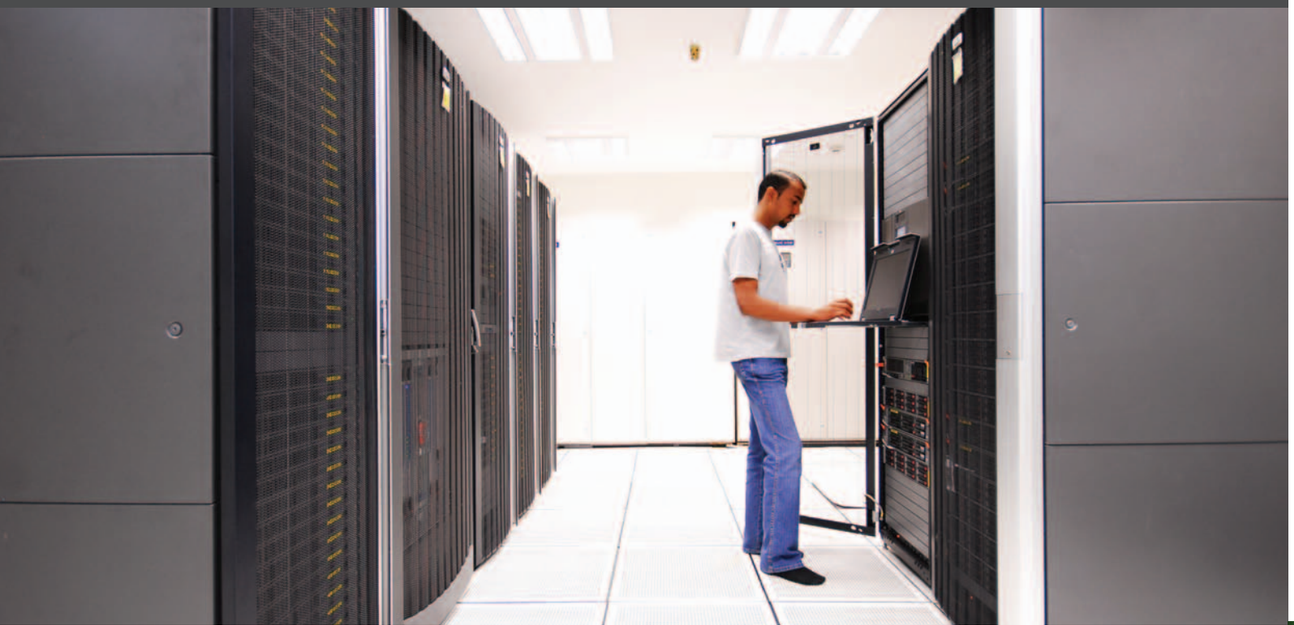
Computer Laboratory (CompLab) is responsible for establishment and maintenance of computer and network facilities at JNCASR, and its connectivity with the rest of the world through internet. Its goal is to continuously evolve the information technology (IT) resources at the Centre that meet the IT requirements of the highly heterogeneous community ranging from Administration, Scientists and Engineers, facilitating cooperation and collaborative interactions amongst them. It interfaces with every Unit and section at JNCASR, seeks inputs from a broad set of users in planning the IT infrastructure. This includes various servers, softwares, local area network (LAN), internet links, multi-media communication over internet and high performance computing (HPC) housed in the Central Facility. In addition, CompLab provides support and services to maintain computing resources in different groups at JNCASR, efficiently through an online ticketing system (http://www/complab).

CompLab hosts email, web, proxy and gateway servers of the Centre, Link-load-balancer, IronPortC150 (a spam-controller), a Firewall and maintains many other servers that cater to Purchase, Canteen and Labrary. An uninterrupted LAN connectivity within the Centre is achieved at 1 Gbps with Optical Fiber Cable (OFC) backbone, CAT-6 network cables and a manageable chasis switch. The centre is connected to internet via 10 Mbps + 25Mbps leased lines from BSNL & HCL Infotech, respectively. As a member of the National Knowledge Network, Complab is expected to



host a link at the band-width of 1 Gbps. Complab maintains HPC resources at a moderate level, and has plans to expand them further. A centralized back-up facility via NAS/SAN helps store critical data from various servers as well as those from the Purchase and Accounts sections. Infrastructural support is given for Windows, Mac and Linux based machines across the Centre.

In addition to the Server and Cluster laboratories, CompLab maintains a 24-hour central computing facility of two terminal rooms with printers and several desktop Linux and Windows PCs running equipped with a wide range of the scientific softwares and databses. Each member of JNCASR has a quota and access to free print-outs from CompLab's high-quality colour and monochrome printers.

In the near future, CompLab plans to further enhance the Email server, acquire Video (both Archival and Live) Streaming solutions.

HEAD
Dr Santosh Ansumali (2012-)
Prof Umesh V Waghmare (2011- 2012)

R&D ASSISTANTS
Vikas Mohan Bajpai, Vishnu Pradeep and Kiran Kumar S

ONLINE SUPPORT ENGINEER (under the Facility Management Contract)
Ashish Purna B

Email: complab@jncasr.ac.in Web: www.jncasr.ac.in/complab

ANIMAL FACILITY

Located in a secluded corner of the campus the Central Animal Facility (CAF) provides an excellent environment for animal care. The facility is equipped for small animal studies. It has rooms for breeding and experiment on mice, rats and rabbits, and a quarantine room, These are temperature- and humidity-regulated rooms with provision of clear-air for care and maintenance of animals. The primary responsibility of the facility is the supply, basic husbandry and quality control of animals used for various research programmes in the centre.

The facility has been registered (No. 201/ CPCSEA) for breeding and experimentation on laboratory animals under the CPCSEA, Government of India. An Institutional Animal Ethics Committee (IAEC) reviews the scientific projects before the initiation of experiment involving animals and ensures compliance of guidelines during the course of the research studies. Animal facility provides investigators with the infrastructure for breeding and experimentation. Procurement of animals from other sources is regulated by the animal facility management team. Personnel working in the facility have received appropriate training with proper handling and husbandry of the laboratory animals.

Veterinarian: Dr R G Prakash

ENDOWED CHAIRS AND HONORARY FACULTY

Many scientific institutions and industrial houses have instituted Endowment Chairs at JNCASR. Eminent scientists in India hold these Chairs at the Centre.

LINUS PAULING RESEARCH PROFESSOR
CNR Rao
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

DS KOTHARI CHAIR
MM Sharma
Emeritus Professor of Eminence, Mumbai University, Mumbai

HINDUSTAN LEVER CHAIR
Prof. S. Chandrasekaran
Indian Institute of Science, Bangalore

DR VIKRAM SARABHAI CHAIR
Kalyan B Sinha
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

HONORARY FACULTY

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Prof KS Valdiya
Prof KB Sinha
Prof S B Kripanidhi (IISc)
Prof Milan Kumar Sanyal (SNP, Kolkata)
Prof Partha Pratim Majumder (ISI, Kolkata)
Prof N Sathyamurthy (IISER, Mohali)
Prof S Ranganathan (IISc)
Prof SK Joshi (NPL)
Dr T Ramasami (DST)
Prof Dipankar Chatterji (IISc)
Prof K VijayRaghavan (NCBS)
Dr P Rama Rao (Hyderabad)
Prof P Balaram (IISc)
Prof S Chandrasekaran (IISc)
Prof MV George (RRL, Tvm.)
Prof DD Sarma (IISc)
Prof S Dattagupta (IISER)
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Prof AK Raychaudhuri (IISc)
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Adjunct Professor (MBGU)
Prof Uday Muthane (Parkinson's Research Centre, Bangalore)

Adjunct Professors (ICMS)
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Prof PM Ajayan (Rice University, USA)
Prof Vinayak P Dravid (Northwestern University, USA)

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Dr Amit Chattopadhya (CCMB)
Prof Satyajit Mayor (NCBS)
Dr LS Shashidhara (IISER, Pune)
Dr K George Thomas (RRL, Tvm.)
Prof Umesh Varshney (IISc)
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Prof. D.D. Sarma SSCU, IISc	Member
Prof. Devang V Khakhar Director, IIT, Mumbai	Member (UGC Nominee)

PRESIDENTS

Prof MRS Rao: 2003 onwards
Prof V Krishnan: 2000 – 2003
Prof CNR Rao: 1989 – 1999

HONORARY FELLOWS

Prof Antony K Cheetam	2012
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Dr. Kapil Sibal	2010
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Prof. S Varadarajan	2006
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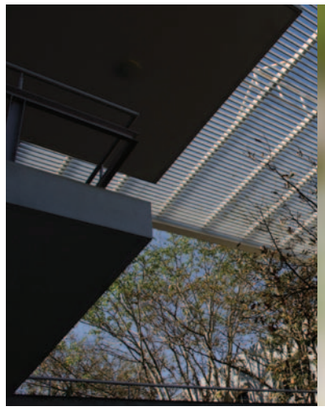
Prof. MM Sharma	2003
Prof. CNR Rao	2000
Mr. NR Narayana Murthy	1999
Prof. C Subramaniam	1998
Prof. Raja Ramanna	1995
Dr. KR Narayanan, Former President of India	1995
Dr. Ashok Ganguly	1995



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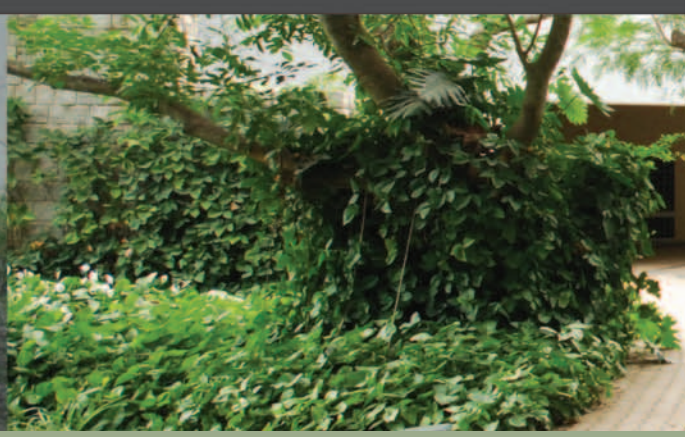

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